Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

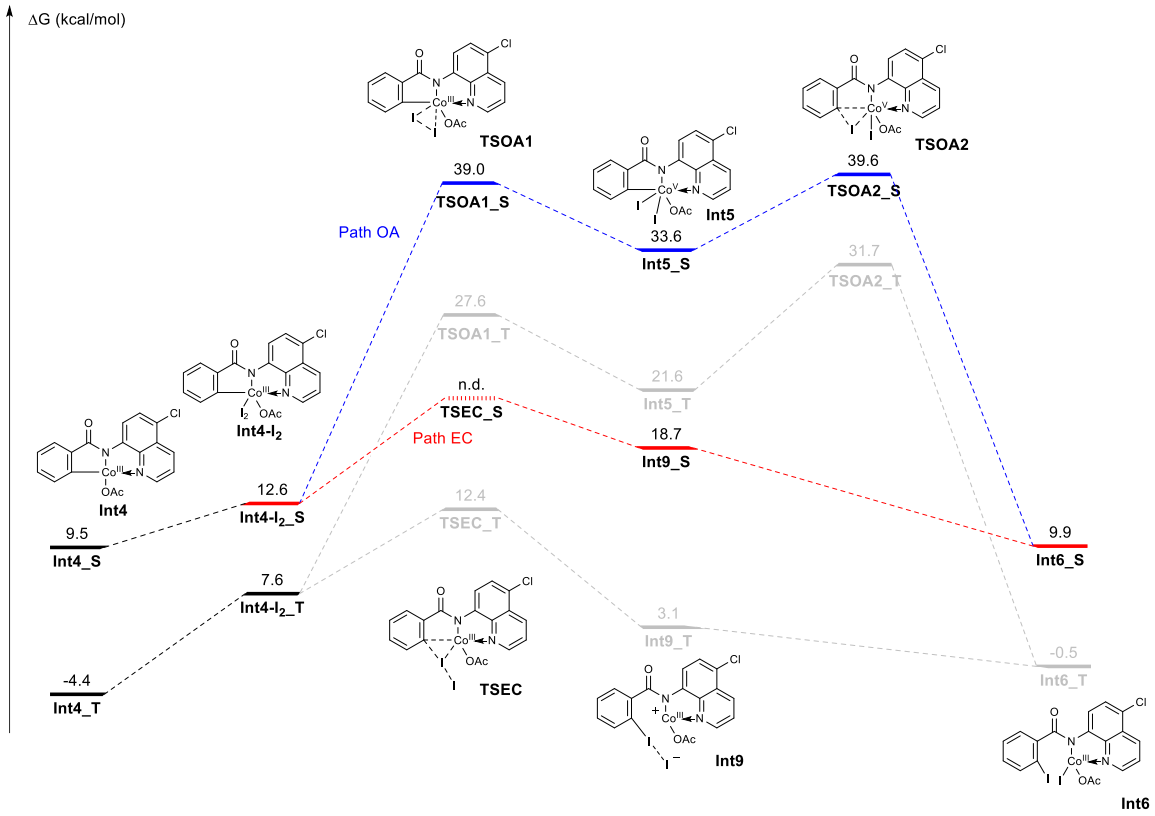
A Computational Study of Cobalt-Catalyzed C-H Iodination Reactions Using a Bidentate Directing Group with Molecular Iodine

Ken Yamazaki, Yadagiri Kommagalla, Yusuke Ano and Naoto Chatani*

Department of Applied Chemistry, Faculty of Engineering, Osaka University,
Suita, Osaka 565-0871, Japan
chatani@chem.eng.osaka-u.ac.jp

Contents

I. Full energy profile of the singlet state iodination pathways

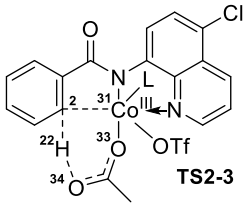


Scheme S1 Computed energy profile of the singlet state iodination process. The triplet state iodination process is also shown in gray lines as a for comparison of the energy differences between singlet and triplet states.

The singlet state iodine-coordinated intermediate **Int4-I_2_S** is less stable than the triplet state, **Int4-I_2_T** by 5.0 kcal/mol. Path OA in the singlet state (blue dodded line) can proceed through the the transition state **TSOA1_S** with an activation energy barrier of 26.4 kcal/mol. The reductive elimination from **Int5_S** to produce the singlet state Co(III) intermediate **Int6_S** requires 6.0 kcal/mol of energy through **TSOA2_S**. As expected, path OA in the singlet state, as well as the triplet state (grey dodded line), is unlikely to participate in the iodination process. Path EC in the singlet state (red dodded line) was also investigated, but it was not possible to locate the transition state geometry of **TSEC_S**. This result is consistent with a previous report on Ni-catalyzed C-H iodination reactions, where the TS geometry using an amide-oxiazoline directing group could be located, but the TS geometry using 8-aminoquinoline directing group could not. **Int9_S** is more unstable than the triplet state, **Int9_T**, and even after the recombination of a cobalt cation and iodine anion in **Int9**, **Int6_S** is still more energetically unstable than **Int6_T**.

II. Effect of effective core potential to the computational models

	B3LYP/6-311+G(d,p)//B3LYP/6-31G(d)	B3LYP/6-311+G(d,p)+SDD//B3LYP/6-31G(d)+Lanl2DZ
Int1_S	0.0	0.0
Int2_S	10.4	10.2
TS2-3_S	14.4	14.4
Int3_S	-0.1	-0.2
Co(31)•••C(2)	2.093 Å	2.099 Å
C(2)•••H(22)	1.274 Å	1.271 Å
H(22)•••O(34)	1.355 Å	1.361 Å
Co(31)•••O(33)	1.892 Å	1.898 Å



TS2-3

Scheme S2 Comparison between DFT results of Gibbs free energies and optimized structure obtained with and without effective core potential of the CMD process. All energies are shown in kcal/mol.

We tested the B3LYP/6-311+G(d,p)//B3LYP/6-31G(d) level of theory as a comparison to the present methodology. The Gibbs free energies of CMD process, as well as bond lengths of the transition state **TS2-3_S** by B3LYP/6-311+G(d,p)//B3LYP/6-31G(d) and B3LYP/6-311+G(d,p)+SDD//B3LYP/6-31G(d) +Lanl2DZ are nealy identical. Thus, the results with and without effective core potential gave similar results.

III. Comparison of energies by various functionals and basis sets

DFT	Basis set	AMLA/CMD	electrophilic cleavage
		$\Delta G_{TS2\text{-}3\_S} - \Delta G_{Int2\_S}$	$\Delta G_{TSEC\_T} - \Delta G_{Int4\text{-}I2\_T}$
B3LYP	6-31G(d) + Lanl2DZ	4.3	6.6
	6-31G(d) + SDD	4.5	6.5
	6-311+G(d,p) + Lanl2DZ	4.1	5.3
	6-311+G(d,p) + SDD	4.2	4.7
	6-311+G(3df,2pd) + Lanl2DZ	4.5	4.9
	6-311+G(3df,2pd) + SDD	4.4	3.5
B3PW91	6-31G(d) + Lanl2DZ	2.4	3.9
	6-31G(d) + SDD	2.5	3.0
	6-311+G(d,p) + Lanl2DZ	2.0	2.6
	6-311+G(d,p) + SDD	2.0	1.3
	6-311+G(3df,2pd) + Lanl2DZ	2.3	1.3
	6-311+G(3df,2pd) + SDD	2.2	-0.2
ωB97XD	6-31G(d) + Lanl2DZ	5.0	7.6
	6-31G(d) + SDD	5.2	8.7
	6-311+G(d,p) + Lanl2DZ	4.7	6.9
	6-311+G(d,p) + SDD	4.8	9.9
	6-311+G(3df,2pd) + Lanl2DZ	5.2	6.8
	6-311+G(3df,2pd) + SDD	5.0	6.7
M06	6-31G(d) + Lanl2DZ	3.6	2.2
	6-31G(d) + SDD	4.0	-0.9
	6-311+G(d,p) + Lanl2DZ	3.8	0.6
	6-311+G(d,p) + SDD	4.1	-2.4
	6-311+G(3df,2pd) + Lanl2DZ	4.1	-1.2
	6-311+G(3df,2pd) + SDD	4.2	-4.1
M06L	6-31G(d) + Lanl2DZ	5.6	9.7
	6-31G(d) + SDD	5.8	8.9
	6-311+G(d,p) + Lanl2DZ	5.9	8.8
	6-311+G(d,p) + SDD	5.9	8.1
	6-311+G(3df,2pd) + Lanl2DZ	6.1	8.0
	6-311+G(3df,2pd) + SDD	6.1	7.0

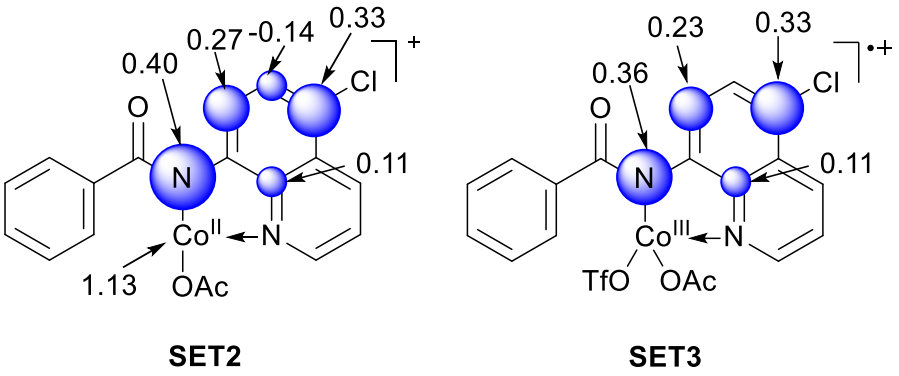
Scheme S3 Comparison of Gibbs free energies of AMLA/CMD process and electrophilic cleavage process by various functionals and basis sets. All energies are shown in kcal/mol.

In order to obtain a more concise and reliable overview of the reaction path, activation energies of singlet AMLA/CMD process and triplet electrophilic cleavage process have been calculated with various density functional approximations. Thermal corrections have been added from the geometry optimizations at the B3LYP/6-31G(d) + Lanl2DZ level of theory.

B3PW91 underestimated the energy for both singlet CMD and triplet electrophilic cleavage pathways. The calculated reaction barriers of singlet CMD process are consistent with B3LYP, ωB97XD, M06, and

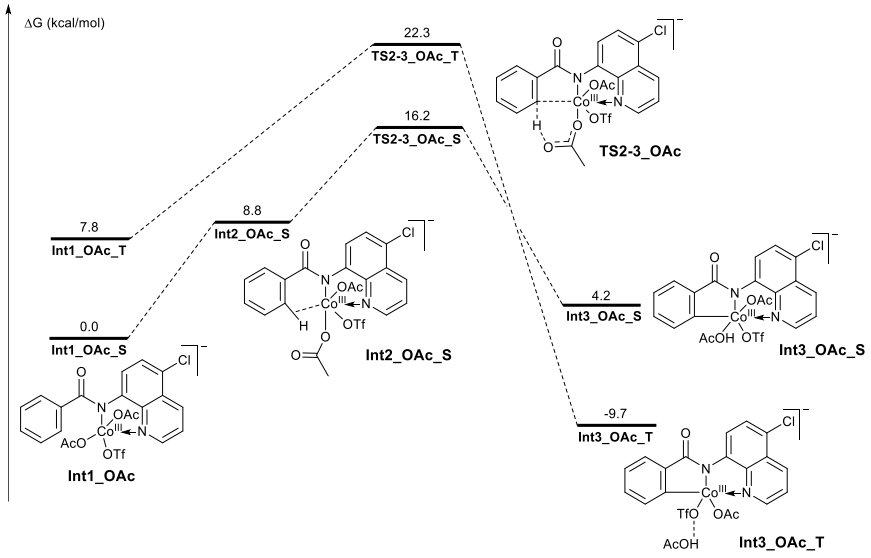
M06L, and ωB97XD and M06L predict slightly larger values. On the other hand, the calculated reaction barriers of triplet electrophilic cleavage process is not consistent with several density functionals and basis sets. Interestingly, M06 functional was unable to evaluate energy on a triplet surface, and even the energies of the transition state calculated with M06 function was reversed. Thus, the present methodologies on the results for triplet surface showed some limitations.[1,2] Further study on the suitability of calculation methods are under investigation.

IV. Spin densities for calculated structures in Scheme 7



Scheme S4 Spin densities of possible intermediates of intra- and intermolecular SET processes in Scheme 7.

V. Possible CMD processes with an anioic acetate ligand



Scheme S5 Possible CMD processes with an anionic acetate ligand.

VI. Energies for calculated structures

Electronic energies, as well as zero point energy (ZPE), enthalpy (H), Gibbs free energy (G), spin contamination ($<S^2>$), and imaginary frequency (Im. Freq.) for all structures calculated at B3LYP/6-31G(d) + Lanl2DZ level of theory are provided. PCM solvent effects were incoorporated for all calculations with dichloroethane as the solvent.

Table S1 Energies for CMD and SET process (in hartrees)

structure	E	ZPE	H	G^o	$<S^2>$	Im. Freq.
Int1_S	-2824.857145	0.370233	0.406354	0.300645	-	-
Int1_T	-2824.835513	0.367819	0.405530	0.292560	2.059	-
Int2_S	-2824.836116	0.369715	0.406491	0.299209	-	-
TS2-3_S	-2824.827536	0.365512	0.401470	0.297462	-	884.60i
TS2-3_T	-2824.812367	0.363047	0.400446	0.289704	2.117	621.64i
Int3_S	-2824.852674	0.370536	0.407025	0.300963	-	-
Int3_T	-2824.854827	0.367968	0.405969	0.292342	2.164	-
MECP	-2824.845962	0.369420	0.406661	0.298092	-	-
entry2_pre	-1874.807996	0.341190	0.371466	0.278572	-	-
entry2_TS	-1874.800488	0.337108	0.366607	0.276339	-	939.52i
entry3_pre	-2127.809378	0.369712	0.402333	0.304819	-	-
entry3_TS	-2127.798474	0.365529	0.397320	0.303155	-	981.18i
entry4_pre	-3557.741451	0.344510	0.384828	0.269021	-	-
entry4_TS	-3557.732193	0.340385	0.379977	0.266605	-	853.58i
entry5_pre	-3557.772134	0.346939	0.387217	0.271094	-	-
entry5_TS	-3557.741215	0.341264	0.380715	0.267326	-	1221.15i
entry6_pre	-2860.752032	0.347126	0.383077	0.277600	-	-
entry6_TS	-2860.740028	0.342595	0.377753	0.275346	-	1009.16i
SET1	-2595.741949	0.306495	0.337554	0.241444	-	-
SET2	-1634.146914	0.276838	0.299563	0.222748	2.036	-
SET3	-2595.531003	0.306463	0.337580	0.241465	1.042	-
OTf^-	-961.5779531	0.027166	0.035277	-0.005342	-	-
Ag_2CO_3	-555.3696793	0.015545	0.022932	-0.019463	-	-
$Ag_2CO_3^{\cdot -}$	-555.4876126	0.015470	0.023689	-0.021395	0.7554	-

Table S2 Energies for iodination process (in hartrees)

structure	E	ZPE	H	G	$<S^2>$	Im. Freq.
Int4_S	-1633.697005	0.265823	0.287578	0.215680	-	-
Int4_T	-1633.709846	0.264573	0.287017	0.211796	2.095	-
AcOH	-229.0875805	0.061820	0.067349	0.034489	-	-
TfOH	-962.0067425	0.038298	0.047099	0.004964	-	-
I_2	-22.77106236	0.000412	0.004308	-0.025550	-	-
Int4-I2_S	-1656.479679	0.266842	0.293266	0.206516	-	-
Int4-I2_T	-1656.488023	0.266441	0.293083	0.203765	2.037	-
TSOA1_T	-1656.453577	0.265357	0.291722	0.204262	2.030	69.07i
Int5_T	-1656.463579	0.265782	0.292580	0.204748	2.034	-
TSOA2_T	-1656.443767	0.264595	0.290996	0.204543	2.138	194.86i
Int6_T	-1656.497589	0.265632	0.292582	0.203531	2.059	-
I·	-11.36411078	0.000000	0.002360	-0.017503	0.7502	-
Int7_D	-1645.104607	0.266096	0.290123	0.211275	0.782	-
TSHD_D	-1645.085419	0.264593	0.288429	0.209795	0.858	205.24i
Int8_D	-1645.108451	0.265381	0.290070	0.207051	0.966	-
TSEC_T	-1656.476683	0.264761	0.291289	0.202866	2.042	79.36i
Int9_T	-1656.491354	0.265769	0.292875	0.201204	2.039	-
TSOA1_S	-1656.434130	0.265381	0.291665	0.205805	-	72.89i
Int5_S	-1656.450081	0.265994	0.292680	0.207252	-	-
TSOA2_S	-1656.435714	0.264825	0.291082	0.206330	-	154.73i
Int6_S	-1656.486241	0.267283	0.293543	0.208564	-	-
Int9_S	-1656.467327	0.266980	0.293483	0.206314	-	-
Int1_OAc_S	-2824.404536	0.357565	0.393986	0.286335	-	-
Int2_OAc_S	-2824.389252	0.357147	0.393672	0.287463	-	-
TS2-3_OAc_S	-2824.375467	0.352654	0.388353	0.285473	-	1125.95i
Int3_OAc_S	-2824.394212	0.357157	0.393859	0.286736	-	-
Int1_OAc_T	-2824.384971	0.355651	0.392832	0.283146	2.081	-
TS2-3_OAc_T	-2824.352706	0.350132	0.387084	0.277654	2.124	858.76i
Int3_OAc_T	-2824.404130	0.355595	0.393281	0.280659	2.104	-

VII. References

1. M. Reiher, *Chimia*, 2009, **63**, 140.

2. A. J. Cohen, P. Mori-Sánchez, W. Yang, *Science* 2008, **321**, 792.

VIII. B3LYP/6-31G(d) + Lanl2DZ-optimized structures of the model compounds

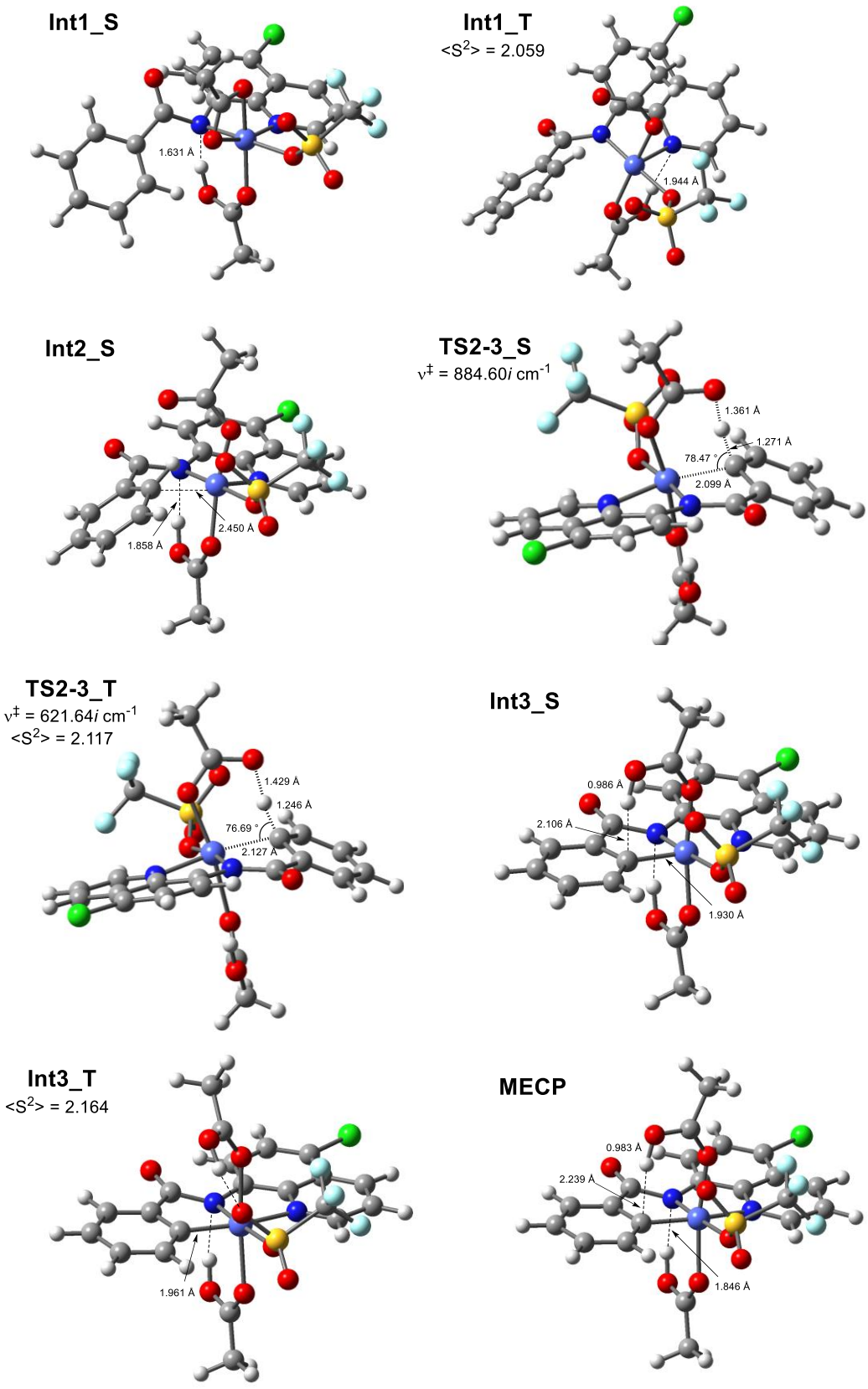
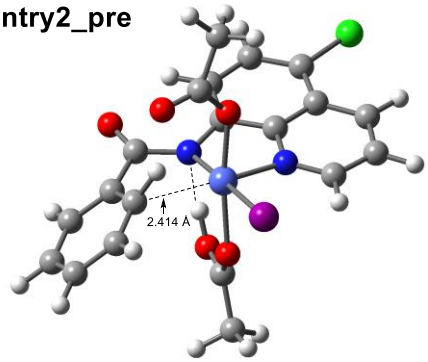


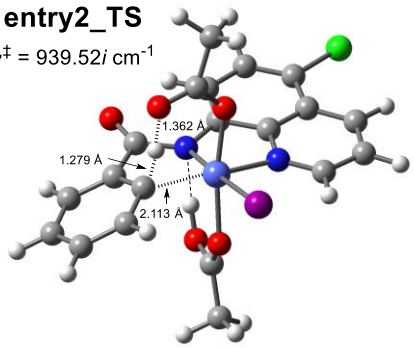
Figure S1 B3LYP/6-31G(d) + Lanl2DZ-optimized structures of the model compounds in Scheme 4.

entry2_pre

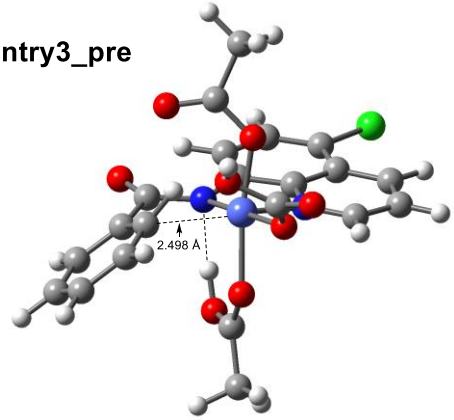


entry2_TS

$\nu^{\ddagger}$ = 939.52*i* cm^{-1}

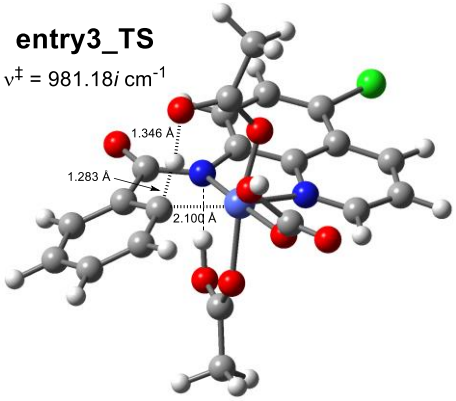


entry3_pre

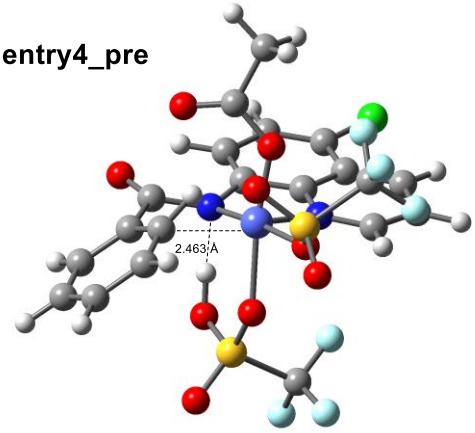


entry3_TS

$\nu^{\ddagger}$ = 981.18*i* cm^{-1}

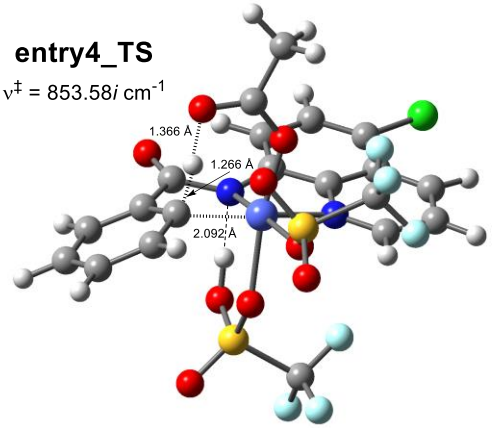


entry4_pre

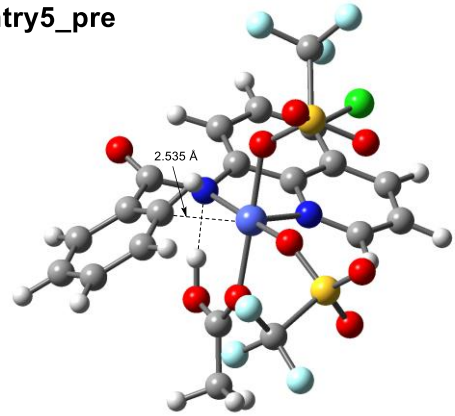


entry4_TS

$\nu^{\ddagger}$ = 853.58*i* cm^{-1}

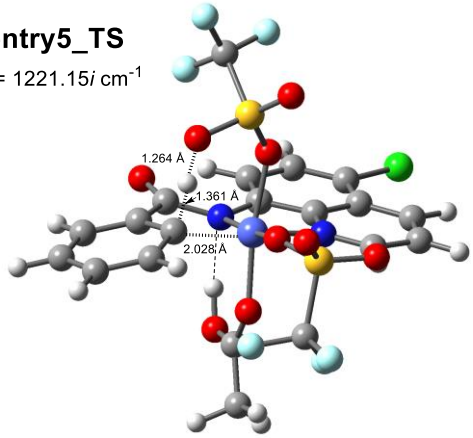


entry5_pre



entry5_TS

$\nu^{\ddagger}$ = 1221.15*i* cm^{-1}



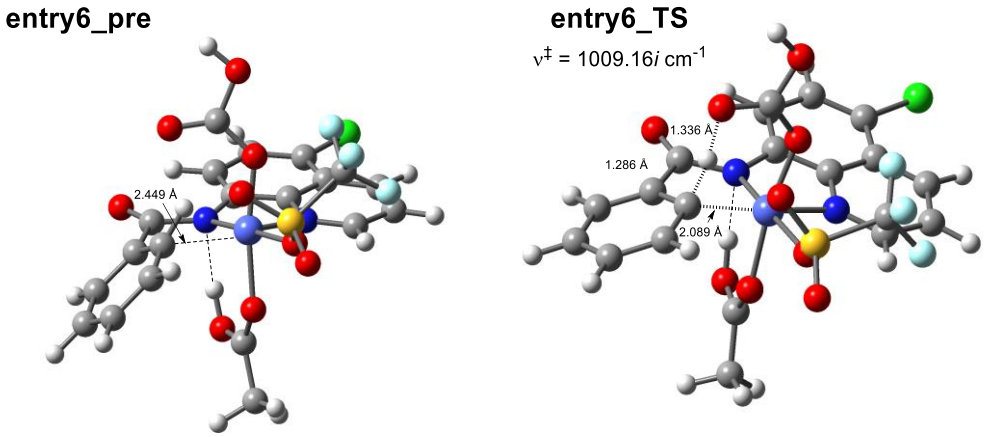
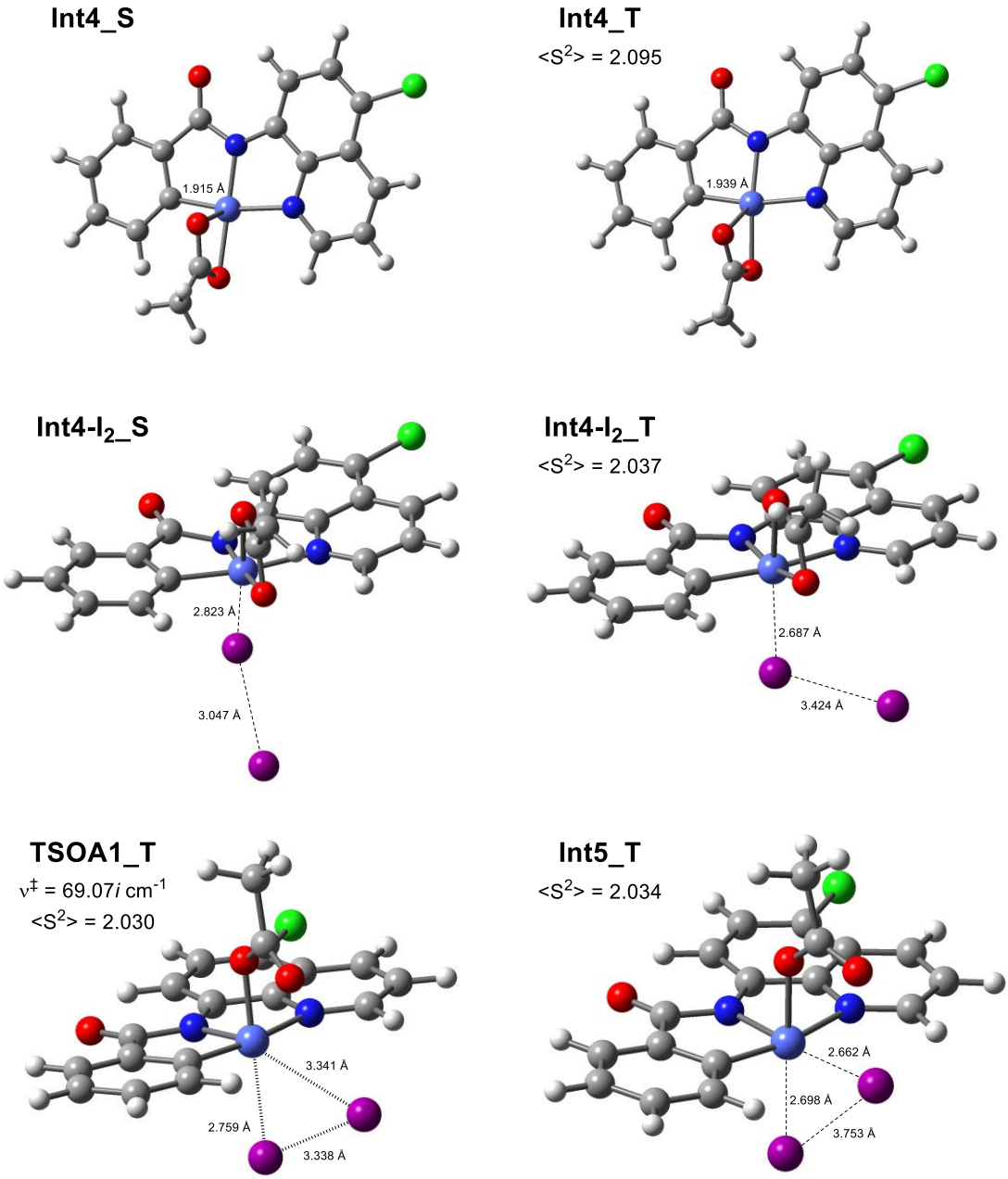


Figure S2 B3LYP/6-31G(d) + Lanl2DZ-optimized structures of the model compounds in Scheme 6.



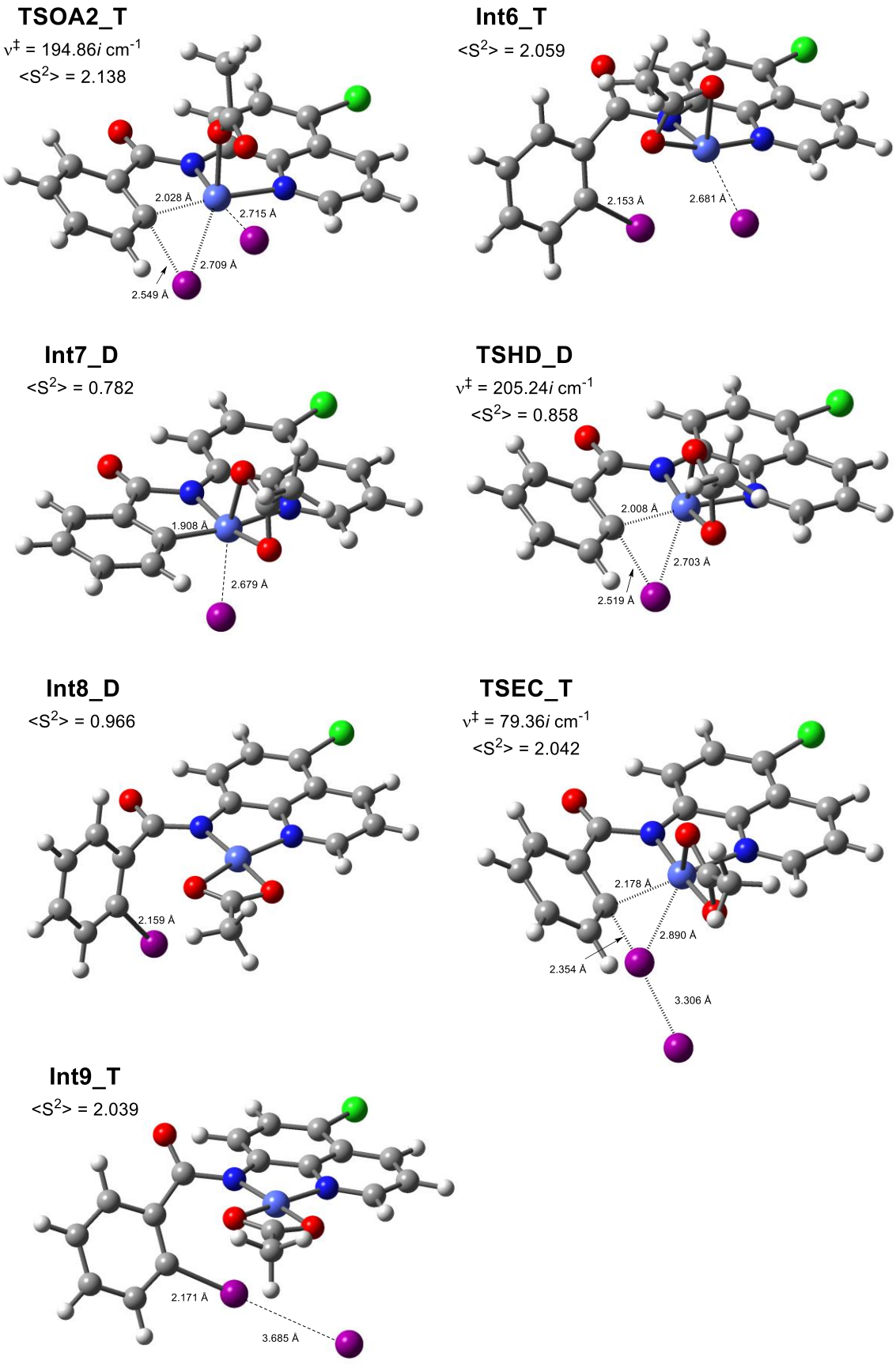


Figure S3 B3LYP/6-31G(d) + Lanl2DZ-optimized structures of the model compounds in Scheme 8

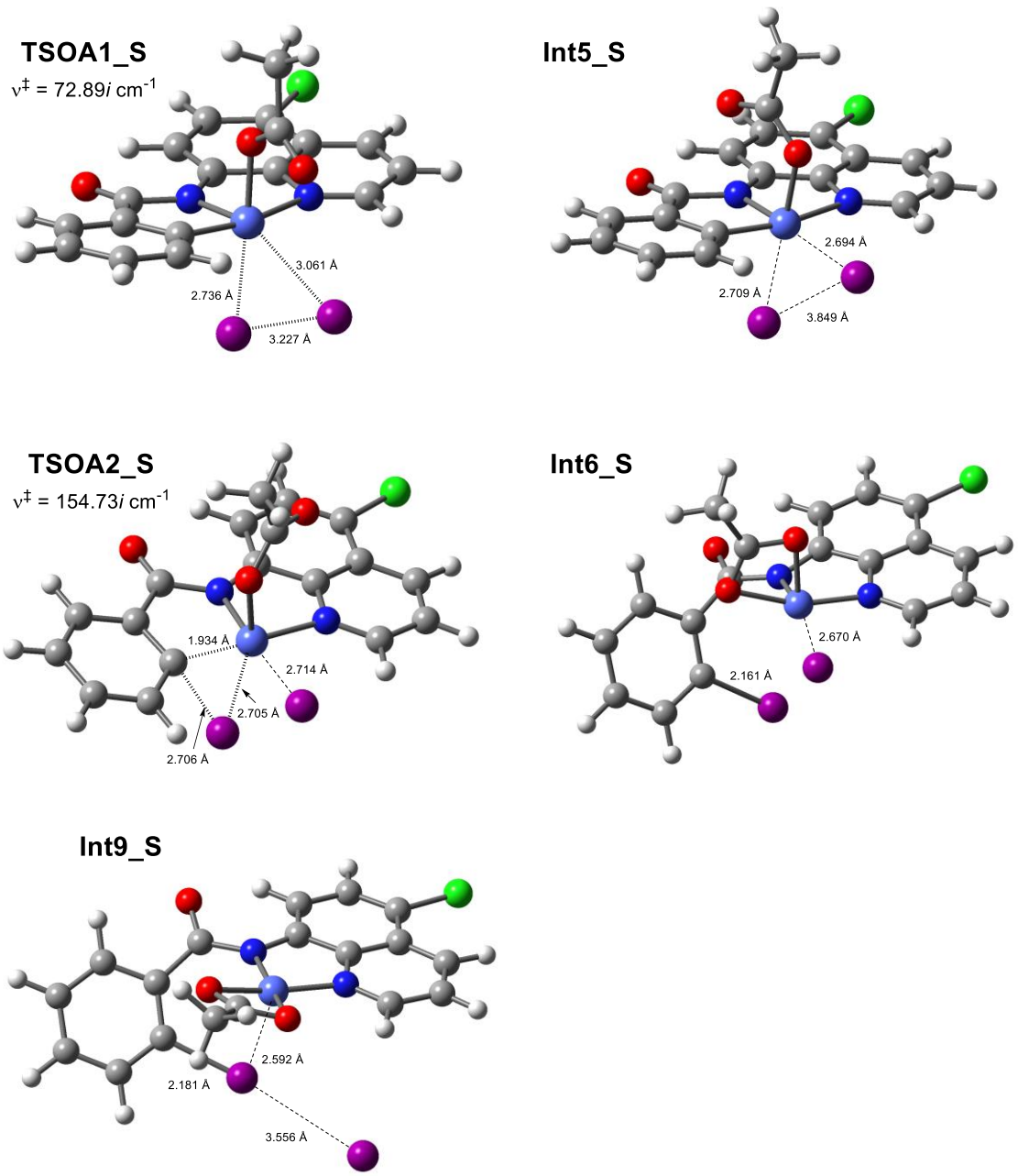


Figure S4 B3LYP/6-31G(d) + Lanl2DZ-optimized structures of the model compounds in Scheme S1.

.

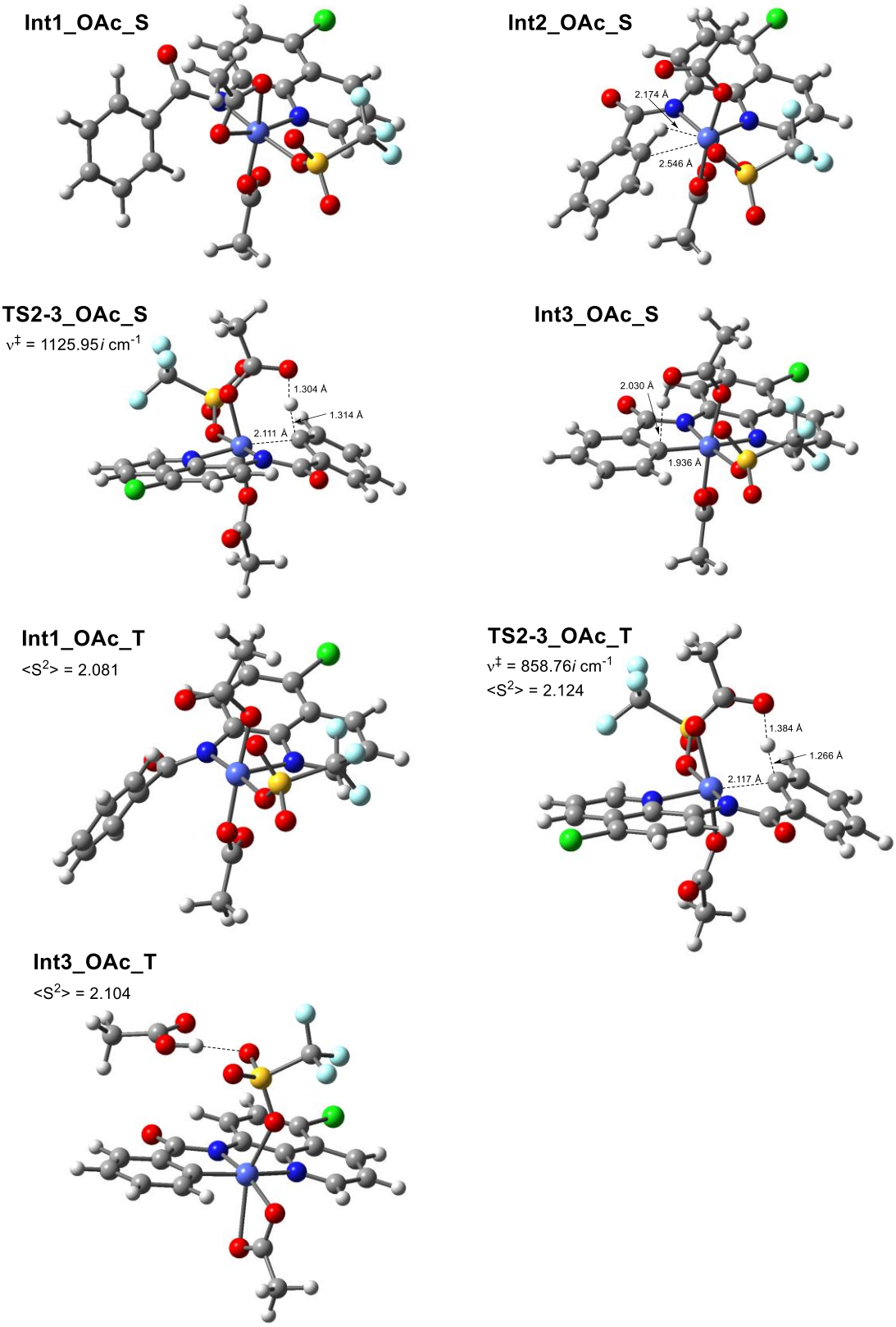


Figure S5 B3LYP/6-31G(d) + Lanl2DZ-optimized structures of the model compounds in Scheme S5.

IX. Cartesian coordinates of the optimized geometries and energies

Scheme 4

Int1_S

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.553429	2.287776	1.119249
2	6	0	-3.501040	1.480147	0.691499
3	6	0	-3.618222	0.723766	-0.484354
4	6	0	-4.812643	0.800590	-1.222802
5	6	0	-5.867911	1.597519	-0.787830
6	6	0	-5.741482	2.343588	0.386863
7	6	0	-2.565481	-0.193610	-1.025095
8	8	0	-2.648001	-0.617865	-2.170780
9	7	0	-1.523843	-0.644181	-0.149154
10	6	0	-0.994128	-1.934059	-0.434281
11	6	0	0.311135	-2.169834	0.068799
12	6	0	-1.669443	-3.008648	-0.994334
13	6	0	0.920692	-3.457287	0.064154
14	6	0	-1.077820	-4.289160	-1.039267
15	6	0	2.163498	-1.206623	1.127435
16	6	0	2.209442	-3.565164	0.643264
17	6	0	0.177482	-4.517252	-0.520161
18	6	0	2.817534	-2.452716	1.182032
19	7	0	0.964906	-1.082887	0.577702
20	17	0	0.862644	-6.132624	-0.585874
21	1	0	-4.442035	2.878077	2.024113
22	1	0	-2.577293	1.485941	1.251325
23	1	0	-4.899254	0.219608	-2.134144
24	1	0	-6.787340	1.637685	-1.364732
25	1	0	-6.561848	2.969338	0.726980
26	1	0	-2.665834	-2.884712	-1.395737
27	1	0	-1.632658	-5.108574	-1.482931
28	1	0	2.617371	-0.302273	1.509990
29	1	0	2.707716	-4.528012	0.660681
30	1	0	3.799400	-2.513346	1.636853
31	27	0	0.009617	0.558606	0.212048

32	6	0	-0.289476	1.739894	-1.738511
33	8	0	0.394283	0.655071	-1.648401
34	8	0	-0.840018	2.097439	-0.642168
35	6	0	-0.476125	2.461953	-3.026103
36	1	0	-0.712970	3.509936	-2.835767
37	1	0	0.426434	2.377918	-3.634069
38	1	0	-1.309277	1.998960	-3.567845
39	8	0	1.606535	1.639344	0.717756
40	16	0	2.483337	2.694420	0.046734
41	8	0	3.021075	3.628013	1.042300
42	8	0	1.933190	3.255783	-1.194594
43	6	0	3.946000	1.674009	-0.493427
44	9	0	4.541718	1.119928	0.573965
45	9	0	3.555758	0.694047	-1.318327
46	9	0	4.830412	2.448621	-1.127569
47	6	0	-1.111646	0.109853	2.893170
48	8	0	-0.406156	0.808286	2.130923
49	8	0	-1.915775	-0.821987	2.463922
50	1	0	-1.894595	-0.805886	1.431089
51	6	0	-1.098221	0.333929	4.373577
52	1	0	-2.065600	0.747969	4.678597
53	1	0	-0.971812	-0.623092	4.887951
54	1	0	-0.300165	1.023384	4.647067

SCF Done: E(RB3LYP) = -2824.85714506 A.U. after 1 cycles

Zero-point correction= 0.370233 (Hartree/Particle)

Thermal correction to Energy= 0.405410

Thermal correction to Enthalpy= 0.406354

Thermal correction to Gibbs Free Energy= 0.300645

Sum of electronic and zero-point Energies= -2824.486912

Sum of electronic and thermal Energies= -2824.451735

Sum of electronic and thermal Enthalpies= -2824.450791

Sum of electronic and thermal Free Energies= -2824.556500

SCF Done: E(RB3LYP) = -2826.23474690 A.U. after 23 cycles

Int1_T

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	3.004245	2.895047	-1.546179
2	6	0	1.710670	2.423399	-1.323046
3	6	0	0.778969	3.225202	-0.646372
4	6	0	1.154202	4.512125	-0.220512
5	6	0	2.447373	4.975338	-0.440578
6	6	0	3.377189	4.164786	-1.101212
7	6	0	-0.617021	2.805213	-0.352002
8	8	0	-1.500956	3.626168	-0.130900
9	7	0	-0.887465	1.410672	-0.212564
10	6	0	-2.181937	0.968557	-0.213393
11	6	0	-2.447599	-0.269437	0.486218
12	6	0	-3.251113	1.581713	-0.894633
13	6	0	-3.733252	-0.874323	0.455027
14	6	0	-4.521841	1.002151	-0.912721
15	6	0	-1.588621	-1.994372	1.788271
16	6	0	-3.893096	-2.107539	1.132584
17	6	0	-4.767036	-0.196991	-0.260704
18	6	0	-2.818575	-2.674590	1.785401
19	7	0	-1.416393	-0.824946	1.178237
20	17	0	-6.365284	-0.883366	-0.335162
21	1	0	3.717690	2.267398	-2.071106
22	1	0	1.404898	1.468794	-1.736136
23	1	0	0.424415	5.130161	0.291618
24	1	0	2.732671	5.965674	-0.097656
25	1	0	4.387242	4.526280	-1.273063
26	1	0	-3.081864	2.495541	-1.445752
27	1	0	-5.321340	1.486161	-1.461864
28	1	0	-0.721184	-2.400750	2.299735
29	1	0	-4.858578	-2.600380	1.128480
30	1	0	-2.910709	-3.623678	2.300634
31	27	0	0.389078	0.064296	0.204929
32	6	0	-0.271322	-0.627958	-2.486729
33	8	0	-0.085541	-1.028399	-1.258865
34	8	0	-0.228679	0.542257	-2.878039
35	6	0	-0.561031	-1.777440	-3.444028
36	1	0	-0.701910	-1.401214	-4.458871
37	1	0	0.271266	-2.488030	-3.423455
38	1	0	-1.458917	-2.316051	-3.122925
39	8	0	1.606685	-1.373487	0.807343

40	16	0	3.024792	-1.583089	0.290521
41	8	0	3.989876	-1.746625	1.387443
42	8	0	3.388039	-0.684304	-0.816304
43	6	0	2.895219	-3.276938	-0.473990
44	9	0	2.421360	-4.154830	0.419783
45	9	0	2.081453	-3.262362	-1.535214
46	9	0	4.109568	-3.679555	-0.871436
47	6	0	0.877272	1.300053	2.841199
48	8	0	1.217657	1.169871	1.657580
49	8	0	-0.217444	0.753151	3.337157
50	1	0	-0.671475	0.237306	2.625735
51	6	0	1.688084	2.079294	3.827557
52	1	0	1.034857	2.681690	4.463505
53	1	0	2.227616	1.374842	4.471167
54	1	0	2.407174	2.708789	3.304102

SCF Done: E(UB3LYP) = -2824.83551340 A.U. after 18 cycles
Zero-point correction= 0.367819 (Hartree/Particle)
Thermal correction to Energy= 0.404586
Thermal correction to Enthalpy= 0.405530
Thermal correction to Gibbs Free Energy= 0.292560
Sum of electronic and zero-point Energies= -2824.467694
Sum of electronic and thermal Energies= -2824.430928
Sum of electronic and thermal Enthalpies= -2824.429984
Sum of electronic and thermal Free Energies= -2824.542953
SCF Done: E(UB3LYP) = -2826.21655775 A.U. after 53 cycles

Int2_S

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.145821	2.321332	-0.347423
2	6	0	1.851665	1.992978	-0.768453
3	6	0	0.859181	2.986979	-0.866843
4	6	0	1.182321	4.313965	-0.575280
5	6	0	2.476114	4.638593	-0.160725
6	6	0	3.454227	3.645475	-0.036787
7	6	0	-0.566482	2.622542	-1.151989

8	8	0	-1.335971	3.340897	-1.781990
9	7	0	-0.937083	1.475157	-0.469028
10	6	0	-2.208378	0.884437	-0.506210
11	6	0	-2.273175	-0.303161	0.272914
12	6	0	-3.369657	1.330492	-1.119184
13	6	0	-3.478699	-1.023516	0.482650
14	6	0	-4.576944	0.614990	-0.945708
15	6	0	-1.041051	-1.801925	1.595832
16	6	0	-3.408915	-2.167484	1.316293
17	6	0	-4.641392	-0.518177	-0.164434
18	6	0	-2.205941	-2.542966	1.876157
19	7	0	-1.095668	-0.726216	0.826381
20	17	0	-6.175793	-1.346365	0.038307
21	1	0	3.905248	1.547903	-0.307074
22	1	0	1.705585	1.025053	-1.263682
23	1	0	0.415625	5.078102	-0.655075
24	1	0	2.721595	5.670916	0.071203
25	1	0	4.458085	3.909292	0.281999
26	1	0	-3.353693	2.229499	-1.718225
27	1	0	-5.474712	0.978949	-1.433361
28	1	0	-0.064693	-2.088969	1.966028
29	1	0	-4.306870	-2.744417	1.507331
30	1	0	-2.132247	-3.413424	2.517488
31	27	0	0.390693	0.257050	0.156142
32	6	0	0.250976	-0.494434	-2.610419
33	8	0	0.226618	-0.842003	-1.340522
34	8	0	0.411698	0.640990	-3.046755
35	6	0	0.067831	-1.701819	-3.519006
36	1	0	0.133878	-1.390127	-4.562723
37	1	0	0.836572	-2.448261	-3.300691
38	1	0	-0.906293	-2.165814	-3.332826
39	8	0	1.723364	-0.997375	0.907702
40	16	0	2.996898	-1.559271	0.275286
41	8	0	4.074735	-1.650911	1.267839
42	8	0	3.314754	-0.974829	-1.035812
43	6	0	2.523461	-3.335060	-0.047603
44	9	0	2.050826	-3.885704	1.079885
45	9	0	1.586171	-3.430746	-0.994420
46	9	0	3.605918	-4.014265	-0.441808
47	6	0	0.085095	2.002577	2.576837

48	8	0	0.715980	1.153728	1.925722
49	8	0	-0.991669	2.605093	2.119728
50	1	0	-1.141373	2.291664	1.187686
51	6	0	0.508942	2.422191	3.948769
52	1	0	0.789464	3.480601	3.929225
53	1	0	-0.332731	2.316303	4.640020
54	1	0	1.352911	1.819995	4.283055

SCF Done: E(RB3LYP) = -2824.83611596 A.U. after 1 cycles
Zero-point correction= 0.369715 (Hartree/Particle)
Thermal correction to Energy= 0.405546
Thermal correction to Enthalpy= 0.406491
Thermal correction to Gibbs Free Energy= 0.299209
Sum of electronic and zero-point Energies= -2824.466401
Sum of electronic and thermal Energies= -2824.430570
Sum of electronic and thermal Enthalpies= -2824.429625
Sum of electronic and thermal Free Energies= -2824.536907
SCF Done: E(RB3LYP) = -2826.21712751 A.U. after 26 cycles

TS2-3_S

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.001517	2.145892	-0.188157
2	6	0	1.660445	1.924450	-0.557956
3	6	0	0.816037	3.052285	-0.727682
4	6	0	1.296723	4.349834	-0.583937
5	6	0	2.634424	4.540869	-0.221835
6	6	0	3.482139	3.445314	-0.020113
7	6	0	-0.627322	2.775985	-0.998842
8	8	0	-1.401597	3.561338	-1.543731
9	7	0	-0.969866	1.549789	-0.458915
10	6	0	-2.227871	0.936674	-0.529547
11	6	0	-2.288183	-0.293650	0.190103
12	6	0	-3.382084	1.402770	-1.141506
13	6	0	-3.493752	-1.035700	0.322753
14	6	0	-4.583672	0.665713	-1.038371
15	6	0	-1.088215	-1.838685	1.467978

16	6	0	-3.436729	-2.225125	1.092272
17	6	0	-4.647028	-0.511078	-0.325481
18	6	0	-2.247501	-2.616088	1.667839
19	7	0	-1.119753	-0.724033	0.757192
20	17	0	-6.175276	-1.372301	-0.213059
21	1	0	3.676130	1.301770	-0.089292
22	1	0	1.601782	1.170818	-1.579892
23	1	0	0.629276	5.193453	-0.731864
24	1	0	3.018370	5.549339	-0.096537
25	1	0	4.520172	3.609517	0.254262
26	1	0	-3.364371	2.336077	-1.686231
27	1	0	-5.475272	1.045203	-1.525628
28	1	0	-0.124450	-2.132132	1.866591
29	1	0	-4.333520	-2.820626	1.222299
30	1	0	-2.182700	-3.520596	2.261720
31	27	0	0.416454	0.380180	0.130424
32	6	0	0.795088	-0.435117	-2.568151
33	8	0	0.234073	-0.669394	-1.440277
34	8	0	1.521711	0.565660	-2.796494
35	6	0	0.559553	-1.461196	-3.649129
36	1	0	0.915002	-1.091883	-4.611563
37	1	0	1.106281	-2.370834	-3.380045
38	1	0	-0.502884	-1.711889	-3.704411
39	8	0	1.751818	-0.899211	0.884543
40	16	0	2.958827	-1.635693	0.321393
41	8	0	3.993665	-1.816942	1.348048
42	8	0	3.381364	-1.166782	-1.006153
43	6	0	2.286257	-3.352893	0.044173
44	9	0	1.751129	-3.826837	1.180169
45	9	0	1.339711	-3.355168	-0.903021
46	9	0	3.276651	-4.166272	-0.336992
47	6	0	-0.052893	1.921088	2.653761
48	8	0	0.651306	1.180816	1.951378
49	8	0	-1.169617	2.474919	2.226262
50	1	0	-1.283755	2.227578	1.272861
51	6	0	0.314867	2.258691	4.064480
52	1	0	0.492518	3.336412	4.142379
53	1	0	-0.519692	2.012562	4.728192
54	1	0	1.208677	1.711371	4.361542

SCF Done: E(RB3LYP) = -2824.82753569   A.U. after   2 cycles
Zero-point correction=   0.365512 (Hartree/Particle)
 Thermal correction to Energy=   0.400525
 Thermal correction to Enthalpy=   0.401470
 Thermal correction to Gibbs Free Energy=   0.297462
 Sum of electronic and zero-point Energies=   -2824.462024
 Sum of electronic and thermal Energies=   -2824.427010
 Sum of electronic and thermal Enthalpies=   -2824.426066
 Sum of electronic and thermal Free Energies=   -2824.530074
SCF Done: E(RB3LYP) = -2826.20867693   A.U. after   23 cycles

TS2-3_T

                         Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.760005	2.336949	-0.375988
2	6	0	1.439631	2.019093	-0.759396
3	6	0	0.489801	3.069896	-0.838879
4	6	0	0.851767	4.394269	-0.617349
5	6	0	2.171712	4.685164	-0.258952
6	6	0	3.119721	3.661646	-0.132663
7	6	0	-0.930765	2.685145	-1.063796
8	8	0	-1.806424	3.440223	-1.475308
9	7	0	-1.129598	1.373423	-0.654308
10	6	0	-2.370509	0.722030	-0.611336
11	6	0	-2.328493	-0.522744	0.080938
12	6	0	-3.585541	1.149400	-1.130483
13	6	0	-3.484041	-1.329377	0.264247
14	6	0	-4.741754	0.353096	-0.971719
15	6	0	-0.979766	-2.025813	1.253653
16	6	0	-3.321286	-2.532418	0.994942
17	6	0	-4.701235	-0.846726	-0.295926
18	6	0	-2.080680	-2.872931	1.490243
19	7	0	-1.110360	-0.895664	0.577591
20	17	0	-6.172258	-1.786860	-0.118740
21	1	0	3.507640	1.552378	-0.337295
22	1	0	1.432160	1.250405	-1.740477
23	1	0	0.103782	5.177393	-0.695024

24	1	0	2.462381	5.714540	-0.069885
25	1	0	4.142112	3.903917	0.141918
26	1	0	-3.648538	2.091182	-1.656079
27	1	0	-5.679459	0.701227	-1.390687
28	1	0	0.016714	-2.268888	1.601981
29	1	0	-4.176772	-3.177679	1.160681
30	1	0	-1.933669	-3.787049	2.053846
31	27	0	0.333641	0.342833	-0.059623
32	6	0	1.041301	-0.600710	-2.754027
33	8	0	0.462199	-0.927189	-1.667109
34	8	0	1.528710	0.544558	-2.977848
35	6	0	1.157529	-1.668848	-3.820319
36	1	0	1.581695	-1.263500	-4.739961
37	1	0	1.801347	-2.467912	-3.437626
38	1	0	0.173197	-2.103272	-4.018844
39	8	0	1.740087	-0.732058	0.879344
40	16	0	3.123019	-1.265281	0.526122
41	8	0	4.035321	-1.192733	1.674625
42	8	0	3.623871	-0.811148	-0.779661
43	6	0	2.785750	-3.086385	0.309035
44	9	0	2.182582	-3.577186	1.404278
45	9	0	1.996725	-3.307624	-0.746877
46	9	0	3.941431	-3.733930	0.129065
47	6	0	-0.309786	2.052610	2.767672
48	8	0	0.421546	1.390160	2.041668
49	8	0	-1.553664	2.407528	2.422484
50	1	0	-1.735169	2.063318	1.526314
51	6	0	0.081196	2.555163	4.126772
52	1	0	0.036897	3.649041	4.139850
53	1	0	-0.628847	2.188087	4.874525
54	1	0	1.088867	2.220004	4.370445

SCF Done: E(UB3LYP) = -2824.81236719 A.U. after 2 cycles

Zero-point correction= 0.363047 (Hartree/Particle)

Thermal correction to Energy= 0.399502

Thermal correction to Enthalpy= 0.400446

Thermal correction to Gibbs Free Energy= 0.289704

Sum of electronic and zero-point Energies= -2824.449320

Sum of electronic and thermal Energies= -2824.412865

Sum of electronic and thermal Enthalpies= -2824.411921

Sum of electronic and thermal Free Energies= -2824.522664

SCF Done: E(UB3LYP) = -2826.19823767 A.U. after 47 cycles

Int3_S

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.983333	2.015579	0.257632
2	6	0	1.619747	1.894119	-0.020724
3	6	0	0.944784	2.979113	-0.609809
4	6	0	1.614214	4.160324	-0.944507
5	6	0	2.977055	4.270470	-0.669272
6	6	0	3.654655	3.204935	-0.067905
7	6	0	-0.511998	2.794902	-0.847754
8	8	0	-1.219326	3.555589	-1.505009
9	7	0	-0.955393	1.654036	-0.175757
10	6	0	-2.218183	1.063765	-0.364078
11	6	0	-2.334039	-0.260976	0.161531
12	6	0	-3.340006	1.644053	-0.939472
13	6	0	-3.567930	-0.974324	0.136526
14	6	0	-4.562724	0.938536	-0.992429
15	6	0	-1.239787	-2.020906	1.225271
16	6	0	-3.577658	-2.269403	0.714200
17	6	0	-4.681902	-0.327315	-0.465618
18	6	0	-2.425001	-2.785041	1.262865
19	7	0	-1.200540	-0.812990	0.690472
20	17	0	-6.236070	-1.150985	-0.540147
21	1	0	3.532982	1.204866	0.724401
22	1	0	2.201104	1.111688	-1.887095
23	1	0	1.062056	4.972720	-1.408696
24	1	0	3.511888	5.182088	-0.919411
25	1	0	4.715530	3.295077	0.150828
26	1	0	-3.278565	2.644091	-1.343422
27	1	0	-5.424273	1.414020	-1.448874
28	1	0	-0.306612	-2.404228	1.621830
29	1	0	-4.497115	-2.844223	0.719333
30	1	0	-2.410282	-3.771531	1.712560
31	27	0	0.424316	0.424770	0.348160

32	6	0	0.994589	-0.182874	-2.537496
33	8	0	0.374374	-0.312548	-1.467966
34	8	0	1.971664	0.668320	-2.737511
35	6	0	0.659157	-1.045562	-3.714058
36	1	0	1.055195	-0.622336	-4.637630
37	1	0	1.115297	-2.027612	-3.543873
38	1	0	-0.422131	-1.180665	-3.779396
39	8	0	1.749523	-0.960903	0.942215
40	16	0	2.899575	-1.719119	0.303315
41	8	0	3.952721	-2.021584	1.281102
42	8	0	3.314823	-1.195980	-1.008200
43	6	0	2.123722	-3.369801	-0.076676
44	9	0	1.622886	-3.921658	1.039095
45	9	0	1.127439	-3.230530	-0.964795
46	9	0	3.042097	-4.194563	-0.588984
47	6	0	-0.147216	1.711600	2.923036
48	8	0	0.487858	0.881625	2.246741
49	8	0	-1.051530	2.513580	2.417587
50	1	0	-1.115498	2.321044	1.431704
51	6	0	0.089225	1.857429	4.393891
52	1	0	0.478582	2.860927	4.595767
53	1	0	-0.860174	1.757209	4.928471
54	1	0	0.800145	1.107635	4.739155

SCF Done: E(RB3LYP) = -2824.85267431 A.U. after 1 cycles

Zero-point correction= 0.370536 (Hartree/Particle)

Thermal correction to Energy= 0.406080

Thermal correction to Enthalpy= 0.407025

Thermal correction to Gibbs Free Energy= 0.300963

Sum of electronic and zero-point Energies= -2824.482139

Sum of electronic and thermal Energies= -2824.446594

Sum of electronic and thermal Enthalpies= -2824.445650

Sum of electronic and thermal Free Energies= -2824.551711

SCF Done: E(RB3LYP) = -2826.23563497 A.U. after 28 cycles

Int3_T

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	2.754567	2.205941	0.336292
2	6	0	1.409943	2.023693	0.034581
3	6	0	0.667738	3.037966	-0.576651
4	6	0	1.275145	4.248500	-0.926676
5	6	0	2.625017	4.439084	-0.637189
6	6	0	3.355646	3.427052	-0.004247
7	6	0	-0.769251	2.754417	-0.816593
8	8	0	-1.532519	3.469294	-1.459432
9	7	0	-1.112966	1.558564	-0.178130
10	6	0	-2.344813	0.903824	-0.348746
11	6	0	-2.364998	-0.456347	0.093119
12	6	0	-3.520106	1.447202	-0.850408
13	6	0	-3.553893	-1.241992	0.052156
14	6	0	-4.700794	0.674520	-0.913172
15	6	0	-1.139300	-2.218600	1.006536
16	6	0	-3.469550	-2.571525	0.534203
17	6	0	-4.725804	-0.628229	-0.471609
18	6	0	-2.272018	-3.055191	1.014110
19	7	0	-1.185740	-0.973053	0.558909
20	17	0	-6.227043	-1.540683	-0.559221
21	1	0	3.343843	1.434608	0.817073
22	1	0	2.891549	-0.205908	-1.960646
23	1	0	0.682214	5.018938	-1.412171
24	1	0	3.110629	5.375248	-0.896775
25	1	0	4.405996	3.583055	0.227840
26	1	0	-3.532219	2.471189	-1.194120
27	1	0	-5.603557	1.125549	-1.310720
28	1	0	-0.176182	-2.568093	1.360243
29	1	0	-4.352912	-3.200262	0.521648
30	1	0	-2.185974	-4.068468	1.389769
31	27	0	0.349053	0.407422	0.360224
32	6	0	1.189087	-0.013879	-2.807630
33	8	0	0.547702	-0.207909	-1.771245
34	8	0	2.507215	0.029060	-2.851014
35	6	0	0.537198	0.186807	-4.146679
36	1	0	0.850362	1.149226	-4.564366
37	1	0	0.868220	-0.594005	-4.838849
38	1	0	-0.547522	0.161041	-4.045212
39	8	0	1.756873	-0.941920	0.961228

40	16	0	3.065148	-1.559128	0.529783
41	8	0	3.941739	-1.890412	1.655165
42	8	0	3.705958	-0.860473	-0.612126
43	6	0	2.519437	-3.195698	-0.173027
44	9	0	1.902891	-3.915988	0.774265
45	9	0	1.669174	-3.003045	-1.188523
46	9	0	3.579469	-3.875528	-0.614689
47	6	0	-0.354872	1.644013	3.150410
48	8	0	0.322629	0.822537	2.526412
49	8	0	-1.258564	2.420776	2.570586
50	1	0	-1.273505	2.209773	1.599416
51	6	0	-0.229749	1.856202	4.629874
52	1	0	0.087825	2.886301	4.822764
53	1	0	-1.204999	1.717737	5.106781
54	1	0	0.496251	1.159604	5.048080

SCF Done: E(UB3LYP) = -2824.85482667 A.U. after 1 cycles
Zero-point correction= 0.367968 (Hartree/Particle)
Thermal correction to Energy= 0.405024
Thermal correction to Enthalpy= 0.405969
Thermal correction to Gibbs Free Energy= 0.292342
Sum of electronic and zero-point Energies= -2824.486859
Sum of electronic and thermal Energies= -2824.449802
Sum of electronic and thermal Enthalpies= -2824.448858
Sum of electronic and thermal Free Energies= -2824.562485
SCF Done: E(UB3LYP) = -2826.24273530 A.U. after 47 cycles

MECP

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.928543	2.080072	0.228573
2	6	0	1.569589	1.946618	-0.055212
3	6	0	0.875529	2.997875	-0.673680
4	6	0	1.534037	4.175523	-1.039199
5	6	0	2.894029	4.308990	-0.760903
6	6	0	3.583876	3.269798	-0.127648
7	6	0	-0.578358	2.786357	-0.904561

8	8	0	-1.297700	3.523777	-1.573509
9	7	0	-0.991522	1.639360	-0.224511
10	6	0	-2.246134	1.028905	-0.392771
11	6	0	-2.341330	-0.287190	0.159736
12	6	0	-3.374145	1.574187	-0.989526
13	6	0	-3.562072	-1.022521	0.143879
14	6	0	-4.583805	0.845942	-1.035252
15	6	0	-1.221715	-2.011604	1.260384
16	6	0	-3.552481	-2.305723	0.746128
17	6	0	-4.684082	-0.408992	-0.479801
18	6	0	-2.393492	-2.792904	1.309401
19	7	0	-1.200353	-0.812314	0.702263
20	17	0	-6.221496	-1.262200	-0.547666
21	1	0	3.483493	1.289499	0.721622
22	1	0	2.213368	1.031560	-1.995079
23	1	0	0.972856	4.966998	-1.528580
24	1	0	3.418054	5.220403	-1.032704
25	1	0	4.642028	3.380492	0.094756
26	1	0	-3.326231	2.564233	-1.418884
27	1	0	-5.449186	1.294589	-1.510867
28	1	0	-0.283015	-2.371892	1.666123
29	1	0	-4.461757	-2.896384	0.757378
30	1	0	-2.365012	-3.770289	1.777940
31	27	0	0.410034	0.438040	0.353499
32	6	0	1.029882	-0.282134	-2.648594
33	8	0	0.419314	-0.404311	-1.581005
34	8	0	2.003032	0.586846	-2.846173
35	6	0	0.724386	-1.152904	-3.829636
36	1	0	1.126069	-0.732267	-4.751975
37	1	0	1.188086	-2.129611	-3.648805
38	1	0	-0.354354	-1.302177	-3.908191
39	8	0	1.771227	-0.928532	0.960847
40	16	0	2.946228	-1.675203	0.355313
41	8	0	3.990887	-1.941133	1.353021
42	8	0	3.372043	-1.163676	-0.957305
43	6	0	2.197183	-3.343588	-0.001724
44	9	0	1.692644	-3.876482	1.122044
45	9	0	1.208939	-3.237745	-0.901646
46	9	0	3.131549	-4.167667	-0.485887
47	6	0	-0.182803	1.799099	3.011389

48	8	0	0.469764	0.955065	2.383801
49	8	0	-1.091587	2.571547	2.446706
50	1	0	-1.136683	2.342657	1.476293
51	6	0	0.002300	2.028033	4.480953
52	1	0	0.362549	3.049099	4.645116
53	1	0	-0.959206	1.930839	4.994159
54	1	0	0.719302	1.313883	4.884992

SCF Done: E(RB3LYP) = -2824.84596205 A.U. after 24 cycles
Zero-point correction= 0.369420 (Hartree/Particle)
Thermal correction to Energy= 0.405717
Thermal correction to Enthalpy= 0.406661
Thermal correction to Gibbs Free Energy= 0.298092
Sum of electronic and zero-point Energies= -2824.476542
Sum of electronic and thermal Energies= -2824.440245
Sum of electronic and thermal Enthalpies= -2824.439301
Sum of electronic and thermal Free Energies= -2824.547870
SCF Done: E(RB3LYP) = -2826.22987393 A.U. after 26 cycles

Scheme 5
entry2_pre

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.774695	0.984812	0.336263
2	6	0	-2.429725	1.116961	0.703447
3	6	0	-1.805680	2.377570	0.653627
4	6	0	-2.541440	3.503435	0.276019
5	6	0	-3.883701	3.366015	-0.082218
6	6	0	-4.497866	2.108303	-0.063261
7	6	0	-0.331879	2.499332	0.886312
8	8	0	0.192304	3.488211	1.395276
9	7	0	0.348764	1.427414	0.338176
10	6	0	1.737784	1.244400	0.394113
11	6	0	2.153277	0.024212	-0.210085
12	6	0	2.711466	2.107998	0.873451
13	6	0	3.524562	-0.306369	-0.389526
14	6	0	4.079066	1.777168	0.742754

15	6	0	1.456449	-1.941439	-1.278594
16	6	0	3.818095	-1.512791	-1.071503
17	6	0	4.480596	0.615859	0.121799
18	6	0	2.792455	-2.309433	-1.529688
19	7	0	1.159726	-0.822368	-0.633360
20	17	0	6.195266	0.273521	-0.048206
21	1	0	-4.250641	0.011181	0.392746
22	1	0	-2.012676	0.300872	1.335666
23	1	0	-2.052027	4.471829	0.245185
24	1	0	-4.451909	4.241123	-0.383993
25	1	0	-5.542416	2.010495	-0.343528
26	1	0	2.422713	3.041382	1.334445
27	1	0	4.824390	2.464750	1.127423
28	1	0	0.626818	-2.568264	-1.579282
29	1	0	4.851632	-1.798037	-1.232403
30	1	0	2.990474	-3.231529	-2.063664
31	27	0	-0.566317	-0.257088	0.020750
32	6	0	-0.531206	-0.931367	2.816943
33	8	0	0.106345	-0.846789	1.676600
34	8	0	-1.691743	-0.578004	3.025028
35	6	0	0.328636	-1.552876	3.908596
36	1	0	-0.162971	-1.440939	4.876576
37	1	0	0.467583	-2.618412	3.694701
38	1	0	1.317714	-1.087026	3.932493
39	6	0	-0.854674	1.016990	-2.656110
40	8	0	-1.193389	0.145255	-1.837631
41	8	0	-0.018184	1.989299	-2.369155
42	1	0	0.222684	1.909464	-1.403260
43	6	0	-1.389273	1.035409	-4.053946
44	1	0	-1.988205	1.941039	-4.197126
45	1	0	-0.556923	1.074627	-4.763233
46	1	0	-2.001383	0.152890	-4.235660
47	53	0	-1.975649	-2.561286	-0.222695

SCF Done: E(RB3LYP) = -1874.80799581 A.U. after 1 cycles

Zero-point correction= 0.341190 (Hartree/Particle)

Thermal correction to Energy= 0.370522

Thermal correction to Enthalpy= 0.371466

Thermal correction to Gibbs Free Energy= 0.278572

Sum of electronic and zero-point Energies= -1874.466806

Sum of electronic and thermal Energies= -1874.437474

Sum of electronic and thermal Enthalpies= -1874.436530

Sum of electronic and thermal Free Energies= -1874.529424

SCF Done: E(RB3LYP) = -1876.00385059 A.U. after 26 cycles

entry2_TS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.594238	0.877597	0.090257
2	6	0	-2.245231	1.057986	0.455527
3	6	0	-1.738300	2.383584	0.479810
4	6	0	-2.553465	3.480981	0.215290
5	6	0	-3.893283	3.271754	-0.124988
6	6	0	-4.409489	1.973745	-0.196924
7	6	0	-0.269463	2.559379	0.692473
8	8	0	0.249719	3.577651	1.147498
9	7	0	0.403398	1.452568	0.205194
10	6	0	1.785027	1.237719	0.298632
11	6	0	2.189172	-0.045429	-0.177149
12	6	0	2.762911	2.126802	0.720704
13	6	0	3.561575	-0.411755	-0.274963
14	6	0	4.126809	1.764018	0.662467
15	6	0	1.494738	-2.093625	-1.054944
16	6	0	3.855691	-1.688035	-0.816196
17	6	0	4.520662	0.540026	0.171238
18	6	0	2.830336	-2.513499	-1.218477
19	7	0	1.190527	-0.909938	-0.546056
20	17	0	6.234635	0.153172	0.090825
21	1	0	-4.007765	-0.125796	0.073349
22	1	0	-2.033239	0.402864	1.533422
23	1	0	-2.133653	4.481873	0.249759
24	1	0	-4.533704	4.122189	-0.341372
25	1	0	-5.450442	1.819561	-0.466605
26	1	0	2.478483	3.104382	1.082776
27	1	0	4.874817	2.473425	0.999586
28	1	0	0.662513	-2.735850	-1.317742
29	1	0	4.888779	-2.002942	-0.912030

30	1	0	3.028491	-3.491314	-1.642472
31	27	0	-0.604196	-0.190926	-0.003525
32	6	0	-0.738950	-0.567411	2.802867
33	8	0	-0.022036	-0.678055	1.750961
34	8	0	-1.887197	-0.046003	2.811495
35	6	0	-0.165256	-1.134109	4.078221
36	1	0	-0.611554	-0.644626	4.945403
37	1	0	-0.403146	-2.203519	4.117205
38	1	0	0.921071	-1.025305	4.091216
39	6	0	-0.728613	0.853725	-2.777610
40	8	0	-1.108774	0.043507	-1.916500
41	8	0	0.092357	1.847648	-2.521526
42	1	0	0.298133	1.826915	-1.542398
43	6	0	-1.193180	0.766597	-4.198301
44	1	0	-1.790459	1.653517	-4.435340
45	1	0	-0.327781	0.762545	-4.867766
46	1	0	-1.790927	-0.132226	-4.345152
47	53	0	-2.020375	-2.530779	-0.102409

SCF Done: E(RB3LYP) = -1874.80048790 A.U. after 1 cycles
Zero-point correction= 0.337108 (Hartree/Particle)
Thermal correction to Energy= 0.365663
Thermal correction to Enthalpy= 0.366607
Thermal correction to Gibbs Free Energy= 0.276339
Sum of electronic and zero-point Energies= -1874.463379
Sum of electronic and thermal Energies= -1874.434825
Sum of electronic and thermal Enthalpies= -1874.433881
Sum of electronic and thermal Free Energies= -1874.524149
SCF Done: E(RB3LYP) = -1875.99554828 A.U. after 23 cycles

entry3_pre

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.057691	-0.303577	-0.182507
2	6	0	-2.746805	-0.479668	-0.632747
3	6	0	-2.222957	-1.767621	-0.833563
4	6	0	-3.040825	-2.880155	-0.617524

5	6	0	-4.354113	-2.704946	-0.176367
6	6	0	-4.861018	-1.420911	0.050822
7	6	0	-0.775311	-1.973321	-1.167690
8	8	0	-0.376947	-2.909931	-1.856324
9	7	0	0.038049	-1.090287	-0.477995
10	6	0	1.437658	-1.074022	-0.548769
11	6	0	2.008006	-0.033054	0.237831
12	6	0	2.300270	-1.945911	-1.198155
13	6	0	3.408788	0.118224	0.420873
14	6	0	3.698800	-1.797611	-1.053127
15	6	0	1.542889	1.818598	1.608303
16	6	0	3.840052	1.169865	1.267761
17	6	0	4.243580	-0.809034	-0.263314
18	6	0	2.916098	2.000651	1.864953
19	7	0	1.128867	0.833098	0.828530
20	17	0	5.988696	-0.693939	-0.096703
21	1	0	-4.443400	0.701777	-0.049982
22	1	0	-2.233790	0.397945	-1.048834
23	1	0	-2.635908	-3.874221	-0.779090
24	1	0	-4.983119	-3.573509	-0.003626
25	1	0	-5.883909	-1.293316	0.392616
26	1	0	1.901209	-2.745844	-1.804788
27	1	0	4.354526	-2.490358	-1.569455
28	1	0	0.775151	2.474240	2.000181
29	1	0	4.900772	1.315345	1.439346
30	1	0	3.226126	2.809646	2.516084
31	27	0	-0.649997	0.585870	0.209491
32	6	0	-0.343316	1.276597	-2.551795
33	8	0	-0.068493	1.536233	-1.293954
34	8	0	-1.042829	0.357433	-2.968387
35	6	0	0.300431	2.294550	-3.485220
36	1	0	0.141509	1.996282	-4.523087
37	1	0	-0.147529	3.279632	-3.315766
38	1	0	1.371767	2.379591	-3.280241
39	8	0	-1.237272	2.240266	0.964621
40	6	0	-1.033021	-1.186408	2.595632
41	8	0	-1.267588	-0.128448	1.988813
42	8	0	-0.332053	-2.171629	2.078520
43	1	0	-0.100392	-1.917101	1.141483
44	6	0	-1.550152	-1.435492	3.977894

45	1	0	-2.314005	-2.219748	3.935505
46	1	0	-0.739213	-1.797139	4.616499
47	1	0	-1.982589	-0.523660	4.388390
48	6	0	-1.973809	3.143995	0.403589
49	8	0	-2.082286	4.306283	0.778256
50	8	0	-2.698338	2.688041	-0.670309
51	1	0	-3.212404	3.448740	-0.992442

SCF Done: E(RB3LYP) = -2127.80937795 A.U. after 1 cycles
Zero-point correction= 0.369712 (Hartree/Particle)
Thermal correction to Energy= 0.401389
Thermal correction to Enthalpy= 0.402333
Thermal correction to Gibbs Free Energy= 0.304819
Sum of electronic and zero-point Energies= -2127.439666
Sum of electronic and thermal Energies= -2127.407989
Sum of electronic and thermal Enthalpies= -2127.407045
Sum of electronic and thermal Free Energies= -2127.504559
SCF Done: E(RB3LYP) = -2129.07137166 A.U. after 26 cycles

entry3_TS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.771752	-0.272913	-0.091126
2	6	0	-2.453832	-0.513365	-0.522402
3	6	0	-2.086121	-1.845208	-0.846143
4	6	0	-3.007617	-2.887159	-0.791379
5	6	0	-4.312639	-2.619156	-0.365548
6	6	0	-4.692285	-1.319587	-0.010276
7	6	0	-0.646940	-2.091074	-1.177975
8	8	0	-0.238349	-3.041420	-1.846526
9	7	0	0.134474	-1.146535	-0.542390
10	6	0	1.527400	-1.036640	-0.624286
11	6	0	2.050401	0.019376	0.183312
12	6	0	2.420979	-1.837037	-1.321584
13	6	0	3.446788	0.255469	0.313827
14	6	0	3.811096	-1.602546	-1.219646
15	6	0	1.525328	1.787459	1.620218

16	6	0	3.844502	1.314372	1.169460
17	6	0	4.314742	-0.596679	-0.424768
18	6	0	2.892980	2.065996	1.823945
19	7	0	1.134930	0.800228	0.833518
20	17	0	6.055859	-0.366467	-0.321315
21	1	0	-4.077259	0.743476	0.136236
22	1	0	-2.131737	0.274709	-1.482031
23	1	0	-2.699902	-3.894194	-1.057127
24	1	0	-5.036589	-3.427349	-0.308915
25	1	0	-5.709880	-1.125694	0.317313
26	1	0	2.051790	-2.647355	-1.934424
27	1	0	4.492828	-2.237867	-1.774841
28	1	0	0.733653	2.374765	2.072187
29	1	0	4.899852	1.526098	1.301199
30	1	0	3.176797	2.879550	2.481856
31	27	0	-0.719664	0.414261	0.213418
32	6	0	-0.807151	1.535296	-2.392468
33	8	0	-0.175775	1.460192	-1.285037
34	8	0	-1.859266	0.889420	-2.647711
35	6	0	-0.255717	2.487619	-3.425453
36	1	0	-0.491408	2.132520	-4.430505
37	1	0	-0.737355	3.461761	-3.281131
38	1	0	0.821609	2.611767	-3.303667
39	8	0	-1.388627	1.986110	1.099438
40	6	0	-0.814880	-1.445290	2.565761
41	8	0	-1.201926	-0.421889	1.984231
42	8	0	-0.005573	-2.327493	2.014377
43	1	0	0.165930	-2.030493	1.080750
44	6	0	-1.243617	-1.775900	3.961853
45	1	0	-1.805408	-2.715712	3.954503
46	1	0	-0.359448	-1.924823	4.589418
47	1	0	-1.861780	-0.974889	4.365608
48	6	0	-2.084228	2.991486	0.694501
49	8	0	-2.215525	4.057292	1.292837
50	8	0	-2.733928	2.790866	-0.500680
51	1	0	-3.229081	3.611041	-0.670621

SCF Done: E(RB3LYP) = -2127.79847362 A.U. after 1 cycles

Zero-point correction= 0.365529 (Hartree/Particle)

Thermal correction to Energy= 0.396376

Thermal correction to Enthalpy= 0.397320
Thermal correction to Gibbs Free Energy= 0.303155
Sum of electronic and zero-point Energies= -2127.432945
Sum of electronic and thermal Energies= -2127.402098
Sum of electronic and thermal Enthalpies= -2127.401153
Sum of electronic and thermal Free Energies= -2127.495318
SCF Done: E(RB3LYP) = -2129.06127716 A.U. after 28 cycles

entry4_pre

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.158516	2.043651	-1.291787
2	6	0	1.957595	1.419907	-1.648496
3	6	0	0.918962	2.158129	-2.246540
4	6	0	1.107369	3.514850	-2.517781
5	6	0	2.310267	4.133208	-2.166896
6	6	0	3.329736	3.404599	-1.545845
7	6	0	-0.430409	1.550074	-2.473628
8	8	0	-1.156100	1.835599	-3.412509
9	7	0	-0.834839	0.790775	-1.360692
10	6	0	-2.027988	0.031350	-1.316718
11	6	0	-2.082724	-0.816388	-0.179659
12	6	0	-3.125777	0.073587	-2.159171
13	6	0	-3.230500	-1.582456	0.154797
14	6	0	-4.270804	-0.703450	-1.864114
15	6	0	-0.903649	-1.602810	1.694010
16	6	0	-3.167564	-2.355152	1.340514
17	6	0	-4.334633	-1.496917	-0.740031
18	6	0	-2.021045	-2.353138	2.107241
19	7	0	-0.955454	-0.865292	0.595163
20	17	0	-5.792199	-2.412258	-0.406540
21	1	0	3.958701	1.452062	-0.860697
22	1	0	1.956121	0.324213	-1.686785
23	1	0	0.305336	4.081888	-2.979311
24	1	0	2.449273	5.190146	-2.373593
25	1	0	4.261514	3.893500	-1.278882
26	1	0	-3.115521	0.707884	-3.033729

27	1	0	-5.120910	-0.657267	-2.535757
28	1	0	0.036593	-1.615563	2.230643
29	1	0	-4.024550	-2.949528	1.636934
30	1	0	-1.953487	-2.936154	3.018133
31	27	0	0.512699	-0.002564	-0.249691
32	6	0	0.727863	-1.689713	-2.546408
33	8	0	0.648473	-1.559851	-1.233734
34	8	0	0.725222	-0.777518	-3.362961
35	6	0	0.839247	-3.154789	-2.940278
36	1	0	0.982321	-3.231590	-4.019254
37	1	0	1.677197	-3.618616	-2.413392
38	1	0	-0.072278	-3.687248	-2.649808
39	8	0	1.819651	-0.698042	1.036996
40	16	0	3.212044	-1.294349	0.799434
41	8	0	4.137689	-0.879133	1.858500
42	8	0	3.662034	-1.196884	-0.596226
43	6	0	2.918819	-3.108595	1.126379
44	9	0	2.302241	-3.258156	2.307310
45	9	0	2.161144	-3.660029	0.174801
46	9	0	4.094460	-3.742533	1.165940
47	8	0	0.541864	1.591637	1.138754
48	8	0	-1.417596	2.854019	0.268527
49	1	0	-1.260844	2.069000	-0.389790
50	6	0	-1.344749	2.380451	2.906430
51	16	0	-0.312180	2.780738	1.391915
52	9	0	-2.205919	3.368190	3.108550
53	9	0	-1.997696	1.239203	2.702343
54	9	0	-0.525393	2.258603	3.942033
55	8	0	0.319835	4.063727	1.618192

SCF Done: E(RB3LYP) = -3557.74145146 A.U. after 1 cycles

Zero-point correction= 0.344510 (Hartree/Particle)

Thermal correction to Energy= 0.383883

Thermal correction to Enthalpy= 0.384828

Thermal correction to Gibbs Free Energy= 0.269021

Sum of electronic and zero-point Energies= -3557.396941

Sum of electronic and thermal Energies= -3557.357568

Sum of electronic and thermal Enthalpies= -3557.356624

Sum of electronic and thermal Free Energies= -3557.472430

SCF Done: E(RB3LYP) = -3559.26242271 A.U. after 26 cycles

entry4_TS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.994894	1.939792	-1.050382
2	6	0	1.749735	1.415045	-1.449501
3	6	0	0.862803	2.263856	-2.163730
4	6	0	1.215583	3.563570	-2.508909
5	6	0	2.460670	4.056945	-2.101293
6	6	0	3.343045	3.252831	-1.371862
7	6	0	-0.497254	1.716291	-2.450900
8	8	0	-1.208664	2.049793	-3.389976
9	7	0	-0.867835	0.853934	-1.414598
10	6	0	-2.032929	0.055303	-1.398110
11	6	0	-2.080229	-0.828213	-0.282120
12	6	0	-3.111526	0.089555	-2.265382
13	6	0	-3.212990	-1.643028	-0.010782
14	6	0	-4.236711	-0.733402	-2.026030
15	6	0	-0.941764	-1.627616	1.594783
16	6	0	-3.159577	-2.456265	1.148877
17	6	0	-4.296364	-1.566251	-0.931318
18	6	0	-2.038879	-2.438026	1.950489
19	7	0	-0.972103	-0.857486	0.520174
20	17	0	-5.729492	-2.546557	-0.669121
21	1	0	3.708377	1.302174	-0.539251
22	1	0	1.919453	0.334842	-2.088436
23	1	0	0.519740	4.186517	-3.062574
24	1	0	2.742451	5.075249	-2.352908
25	1	0	4.307390	3.648464	-1.067233
26	1	0	-3.101033	0.753954	-3.117797
27	1	0	-5.071999	-0.693801	-2.716553
28	1	0	-0.025217	-1.618576	2.172083
29	1	0	-4.003668	-3.090183	1.396479
30	1	0	-1.978112	-3.049708	2.843228
31	27	0	0.541406	0.116434	-0.340621
32	6	0	1.341204	-1.596673	-2.453365
33	8	0	0.623281	-1.429438	-1.399270

34	8	0	2.053328	-0.701634	-2.967399
35	6	0	1.300153	-2.980774	-3.050895
36	1	0	1.784803	-2.986697	-4.027529
37	1	0	1.828667	-3.658999	-2.373059
38	1	0	0.266182	-3.324926	-3.133345
39	8	0	1.839749	-0.592713	0.968569
40	16	0	3.167056	-1.338776	0.862175
41	8	0	4.070077	-0.963624	1.956271
42	8	0	3.712293	-1.387636	-0.501125
43	6	0	2.660440	-3.089484	1.256542
44	9	0	2.061886	-3.135468	2.456003
45	9	0	1.806647	-3.560168	0.337798
46	9	0	3.741743	-3.873517	1.282211
47	8	0	0.469566	1.646034	1.132216
48	8	0	-1.572028	2.829305	0.330583
49	1	0	-1.387399	2.085691	-0.352046
50	6	0	-1.421480	2.290260	2.952015
51	16	0	-0.436826	2.780140	1.431963
52	9	0	-2.294609	3.250891	3.223608
53	9	0	-2.058582	1.148173	2.712741
54	9	0	-0.571385	2.137739	3.958947
55	8	0	0.125577	4.091865	1.679504

SCF Done: E(RB3LYP) = -3557.73219256 A.U. after 1 cycles

Zero-point correction= 0.340385 (Hartree/Particle)

Thermal correction to Energy= 0.379033

Thermal correction to Enthalpy= 0.379977

Thermal correction to Gibbs Free Energy= 0.266605

Sum of electronic and zero-point Energies= -3557.391808

Sum of electronic and thermal Energies= -3557.353160

Sum of electronic and thermal Enthalpies= -3557.352216

Sum of electronic and thermal Free Energies= -3557.465587

SCF Done: E(RB3LYP) = -3559.25393180 A.U. after 26 cycles

entry5_pre

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	3.193385	-0.987408	2.103459
2	6	0	1.796818	-1.060838	1.990166
3	6	0	1.148889	-2.311884	2.037194
4	6	0	1.898433	-3.473580	2.245205
5	6	0	3.285926	-3.389968	2.366950
6	6	0	3.935693	-2.151416	2.283877
7	6	0	-0.320813	-2.426483	1.771064
8	8	0	-1.061676	-3.171176	2.403699
9	7	0	-0.705107	-1.701050	0.652650
10	6	0	-2.037034	-1.539051	0.225685
11	6	0	-2.144680	-0.632429	-0.858948
12	6	0	-3.183820	-2.180528	0.665556
13	6	0	-3.364799	-0.396283	-1.545181
14	6	0	-4.418786	-1.931957	0.023724
15	6	0	-0.962599	0.819973	-2.279976
16	6	0	-3.322128	0.483009	-2.655405
17	6	0	-4.513097	-1.079237	-1.053995
18	6	0	-2.130507	1.065329	-3.028270
19	7	0	-0.991419	0.006471	-1.234915
20	17	0	-6.064506	-0.837269	-1.834776
21	1	0	3.682022	-0.020174	2.072532
22	1	0	1.222812	-0.138285	2.074571
23	1	0	1.394158	-4.433532	2.290513
24	1	0	3.866162	-4.294986	2.520641
25	1	0	5.015982	-2.099139	2.377686
26	1	0	-3.133513	-2.878397	1.488552
27	1	0	-5.306614	-2.440055	0.383661
28	1	0	-0.012313	1.275162	-2.530767
29	1	0	-4.231170	0.687969	-3.209633
30	1	0	-2.071512	1.731780	-3.880635
31	8	0	-0.533106	0.801828	1.306906
32	16	0	-0.668064	2.350657	1.336977
33	8	0	-0.916501	2.945752	0.021120
34	8	0	0.310459	2.973400	2.230836
35	6	0	-2.303097	2.415117	2.234904
36	9	0	-3.248817	1.816573	1.503544
37	9	0	-2.211762	1.805266	3.418803
38	9	0	-2.641633	3.693577	2.424485
39	8	0	1.478055	-1.292417	-1.193599
40	6	0	1.349712	-2.420178	-1.714202

41	27	0	0.402661	-0.267015	0.027731
42	8	0	0.390363	-3.252495	-1.400668
43	1	0	-0.145369	-2.848274	-0.662089
44	6	0	2.311571	-2.891914	-2.754703
45	1	0	2.718628	-3.864295	-2.462393
46	1	0	1.774996	-3.026408	-3.700172
47	1	0	3.110208	-2.162310	-2.879930
48	8	0	1.638384	1.235936	-0.246902
49	16	0	2.506153	1.825129	-1.361355
50	8	0	2.703643	3.262713	-1.160936
51	8	0	2.132108	1.355216	-2.704485
52	6	0	4.182529	1.076975	-1.021117
53	9	0	4.603219	1.437584	0.198150
54	9	0	4.144825	-0.258349	-1.084422
55	9	0	5.050068	1.528668	-1.931434

SCF Done: E(RB3LYP) = -3557.77213383 A.U. after 1 cycles
Zero-point correction= 0.346939 (Hartree/Particle)
Thermal correction to Energy= 0.386273
Thermal correction to Enthalpy= 0.387217
Thermal correction to Gibbs Free Energy= 0.271094
Sum of electronic and zero-point Energies= -3557.425195
Sum of electronic and thermal Energies= -3557.385861
Sum of electronic and thermal Enthalpies= -3557.384917
Sum of electronic and thermal Free Energies= -3557.501040
SCF Done: E(RB3LYP) = -3559.29647652 A.U. after 28 cycles

entry5_TS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.728091	1.511085	1.474949
2	6	0	1.335154	1.404477	1.269225
3	6	0	0.471649	1.971464	2.243125
4	6	0	0.963369	2.716114	3.308027
5	6	0	2.349178	2.858109	3.453110
6	6	0	3.227211	2.249501	2.550811
7	6	0	-0.977102	1.628968	2.128142

8	8	0	-1.885693	2.260356	2.658164
9	7	0	-1.118568	0.437426	1.423395
10	6	0	-2.354332	-0.112679	1.032240
11	6	0	-2.234502	-1.184167	0.100868
12	6	0	-3.616856	0.230913	1.491681
13	6	0	-3.366790	-1.928802	-0.335477
14	6	0	-4.752742	-0.481979	1.048091
15	6	0	-0.780456	-2.471295	-1.195618
16	6	0	-3.131065	-2.999199	-1.234259
17	6	0	-4.637038	-1.535245	0.169801
18	6	0	-1.848222	-3.273379	-1.649526
19	7	0	-0.973340	-1.465167	-0.356540
20	17	0	-6.081005	-2.403573	-0.330577
21	1	0	3.407792	1.067380	0.755474
22	1	0	1.275093	2.095907	0.098814
23	1	0	0.275655	3.148852	4.028205
24	1	0	2.745232	3.433381	4.284918
25	1	0	4.299753	2.352994	2.685640
26	1	0	-3.732114	1.041117	2.196756
27	1	0	-5.730751	-0.195880	1.419392
28	1	0	0.232983	-2.635519	-1.543574
29	1	0	-3.965842	-3.593914	-1.588062
30	1	0	-1.641477	-4.086915	-2.335499
31	8	0	-0.523677	1.058321	-1.118451
32	16	0	0.130382	2.209325	-1.845050
33	8	0	0.497801	2.002273	-3.236617
34	8	0	1.221516	2.794742	-0.952247
35	6	0	-1.216676	3.506099	-1.804416
36	9	0	-2.276133	3.048824	-2.465920
37	9	0	-1.547203	3.751911	-0.537494
38	9	0	-0.768269	4.619285	-2.377231
39	8	0	1.199515	-1.337204	1.433828
40	6	0	0.880139	-1.818989	2.539296
41	27	0	0.337046	-0.060117	0.282966
42	8	0	-0.178439	-1.443035	3.209296
43	1	0	-0.642360	-0.725345	2.683950
44	6	0	1.719947	-2.874054	3.184550
45	1	0	2.136141	-2.478151	4.117034
46	1	0	1.092532	-3.733284	3.440016
47	1	0	2.523084	-3.173899	2.513714

48	8	0	1.917910	-0.248278	-0.947798
49	16	0	2.766797	-1.152984	-1.819776
50	8	0	3.801913	-0.382428	-2.517032
51	8	0	1.995910	-2.130589	-2.606563
52	6	0	3.706039	-2.193925	-0.585476
53	9	0	4.195405	-1.434839	0.403612
54	9	0	2.908220	-3.132982	-0.055661
55	9	0	4.724157	-2.802361	-1.203234

SCF Done: E(RB3LYP) = -3557.74121497 A.U. after 1 cycles
Zero-point correction= 0.341264 (Hartree/Particle)
Thermal correction to Energy= 0.379771
Thermal correction to Enthalpy= 0.380715
Thermal correction to Gibbs Free Energy= 0.267326
Sum of electronic and zero-point Energies= -3557.399951
Sum of electronic and thermal Energies= -3557.361444
Sum of electronic and thermal Enthalpies= -3557.360500
Sum of electronic and thermal Free Energies= -3557.473889
SCF Done: E(RB3LYP) = -3559.26615790 A.U. after 26 cycles

entry6_pre

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.179022	2.273492	-0.325986
2	6	0	1.885369	1.960038	-0.763332
3	6	0	0.902666	2.965897	-0.857773
4	6	0	1.235447	4.286325	-0.548584
5	6	0	2.528600	4.594072	-0.119259
6	6	0	3.496512	3.590479	0.003013
7	6	0	-0.526398	2.619632	-1.149050
8	8	0	-1.284541	3.343365	-1.785470
9	7	0	-0.913696	1.480721	-0.460224
10	6	0	-2.191188	0.900746	-0.500733
11	6	0	-2.268600	-0.284877	0.279176
12	6	0	-3.345784	1.356638	-1.118257
13	6	0	-3.480526	-0.995329	0.484614
14	6	0	-4.559899	0.651872	-0.948189

15	6	0	-1.052363	-1.797015	1.603014
16	6	0	-3.422654	-2.140943	1.316828
17	6	0	-4.636807	-0.480079	-0.166285
18	6	0	-2.224465	-2.528129	1.878892
19	7	0	-1.096886	-0.719010	0.836264
20	17	0	-6.178393	-1.294710	0.031672
21	1	0	3.930736	1.492537	-0.289041
22	1	0	1.739688	1.002021	-1.274598
23	1	0	0.476490	5.058475	-0.624917
24	1	0	2.781268	5.621410	0.126579
25	1	0	4.499538	3.841618	0.334221
26	1	0	-3.319847	2.254683	-1.718455
27	1	0	-5.452730	1.023144	-1.439303
28	1	0	-0.079196	-2.093943	1.973514
29	1	0	-4.325860	-2.710796	1.504176
30	1	0	-2.159629	-3.400800	2.518109
31	27	0	0.401008	0.249142	0.168208
32	6	0	0.217551	-0.482564	-2.583219
33	8	0	0.224775	-0.850463	-1.333816
34	8	0	0.421013	0.631219	-3.055388
35	8	0	1.714882	-1.024562	0.910405
36	16	0	2.977570	-1.605408	0.268790
37	8	0	4.041500	-1.753827	1.269341
38	8	0	3.321843	-0.987889	-1.020362
39	6	0	2.460663	-3.357800	-0.114921
40	9	0	1.906796	-3.910488	0.974716
41	9	0	1.581727	-3.401539	-1.115078
42	9	0	3.542998	-4.066592	-0.456368
43	6	0	0.110599	1.986514	2.573145
44	8	0	0.730016	1.127416	1.920989
45	8	0	-0.954429	2.606615	2.118001
46	1	0	-1.110697	2.299164	1.184190
47	6	0	0.544606	2.393514	3.945079
48	1	0	0.842625	3.447155	3.928041
49	1	0	-0.297761	2.299427	4.637182
50	1	0	1.378903	1.776045	4.275559
51	8	0	-0.046610	-1.556077	-3.375679
52	1	0	-0.010493	-1.226070	-4.290866

SCF Done: E(RB3LYP) = -2860.75203153 A.U. after 1 cycles

Zero-point correction= 0.347126 (Hartree/Particle)
Thermal correction to Energy= 0.382133
Thermal correction to Enthalpy= 0.383077
Thermal correction to Gibbs Free Energy= 0.277600
Sum of electronic and zero-point Energies= -2860.404906
Sum of electronic and thermal Energies= -2860.369899
Sum of electronic and thermal Enthalpies= -2860.368954
Sum of electronic and thermal Free Energies= -2860.474431
SCF Done: E(RB3LYP) = -2862.15434172 A.U. after 29 cycles

entry6_TS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.023735	2.098094	-0.141968
2	6	0	1.678610	1.896848	-0.513290
3	6	0	0.853850	3.040802	-0.682433
4	6	0	1.356557	4.329947	-0.545371
5	6	0	2.698578	4.498549	-0.186505
6	6	0	3.527610	3.389577	0.018629
7	6	0	-0.593990	2.787649	-0.954179
8	8	0	-1.355487	3.586310	-1.496698
9	7	0	-0.954689	1.563897	-0.419147
10	6	0	-2.218311	0.962383	-0.507511
11	6	0	-2.293113	-0.280868	0.187863
12	6	0	-3.364375	1.450243	-1.117168
13	6	0	-3.505926	-1.014691	0.298833
14	6	0	-4.573208	0.722505	-1.034626
15	6	0	-1.113011	-1.865422	1.435945
16	6	0	-3.463252	-2.220946	1.042463
17	6	0	-4.651066	-0.466890	-0.344651
18	6	0	-2.280201	-2.636100	1.613686
19	7	0	-1.131529	-0.734390	0.750941
20	17	0	-6.187451	-1.315956	-0.256927
21	1	0	3.684613	1.243750	-0.039295
22	1	0	1.638289	1.180668	-1.581169
23	1	0	0.703907	5.184638	-0.695564
24	1	0	3.100285	5.500633	-0.065851

25	1	0	4.568643	3.536889	0.290978
26	1	0	-3.335115	2.393003	-1.644816
27	1	0	-5.458446	1.119302	-1.519647
28	1	0	-0.153635	-2.177297	1.831262
29	1	0	-4.365985	-2.810905	1.155348
30	1	0	-2.226308	-3.554665	2.186677
31	27	0	0.419312	0.367834	0.149128
32	6	0	0.786253	-0.375533	-2.559860
33	8	0	0.224647	-0.649529	-1.453736
34	8	0	1.537758	0.612513	-2.786077
35	8	0	1.740523	-0.938755	0.873781
36	16	0	2.933964	-1.679546	0.285846
37	8	0	3.977243	-1.887959	1.298730
38	8	0	3.348488	-1.189476	-1.036855
39	6	0	2.235588	-3.381942	-0.013297
40	9	0	1.714934	-3.870394	1.123999
41	9	0	1.276081	-3.351121	-0.942678
42	9	0	3.210427	-4.199874	-0.425270
43	6	0	-0.033835	1.861647	2.684817
44	8	0	0.662088	1.123354	1.969701
45	8	0	-1.139728	2.439842	2.266983
46	1	0	-1.256339	2.213256	1.307513
47	6	0	0.340651	2.165473	4.101030
48	1	0	0.545837	3.236967	4.196156
49	1	0	-0.500944	1.930216	4.759653
50	1	0	1.220019	1.590993	4.389720
51	8	0	0.514640	-1.235632	-3.546501
52	1	0	0.999296	-0.942293	-4.339280

SCF Done: E(RB3LYP) = -2860.74002799 A.U. after 2 cycles

Zero-point correction= 0.342595 (Hartree/Particle)

Thermal correction to Energy= 0.376809

Thermal correction to Enthalpy= 0.377753

Thermal correction to Gibbs Free Energy= 0.275346

Sum of electronic and zero-point Energies= -2860.397433

Sum of electronic and thermal Energies= -2860.363219

Sum of electronic and thermal Enthalpies= -2860.362275

Sum of electronic and thermal Free Energies= -2860.464682

SCF Done: E(RB3LYP) = -2862.14236258 A.U. after 26 cycles

Scheme 7

SET1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.715524	-3.883735	-2.335528
2	6	0	0.705483	-3.187610	-1.668561
3	6	0	0.347296	-3.545291	-0.359896
4	6	0	0.990073	-4.628916	0.257962
5	6	0	2.006234	-5.312611	-0.403379
6	6	0	2.373732	-4.938621	-1.701004
7	6	0	-0.766315	-2.867516	0.370409
8	8	0	-1.484560	-3.496963	1.145258
9	7	0	-0.981786	-1.518969	0.053997
10	6	0	-2.238560	-0.930970	0.196811
11	6	0	-2.266177	0.423028	-0.243796
12	6	0	-3.444943	-1.499649	0.596959
13	6	0	-3.461012	1.185972	-0.336897
14	6	0	-4.642264	-0.754318	0.531930
15	6	0	-0.971643	2.182580	-1.085265
16	6	0	-3.347484	2.501723	-0.846045
17	6	0	-4.662777	0.546188	0.076417
18	6	0	-2.114871	2.987845	-1.230943
19	7	0	-1.056220	0.948284	-0.601456
20	17	0	-6.183983	1.418145	0.005182
21	1	0	1.980747	-3.606666	-3.351775
22	1	0	0.170647	-2.392628	-2.179741
23	1	0	0.691604	-4.915111	1.261488
24	1	0	2.513190	-6.137608	0.088969
25	1	0	3.164049	-5.475844	-2.217830
26	1	0	-3.473705	-2.520634	0.947321
27	1	0	-5.567817	-1.225301	0.844870
28	1	0	0.015429	2.536338	-1.350123
29	1	0	-4.234327	3.119278	-0.935151
30	1	0	-2.007497	3.988408	-1.633209
31	27	0	0.382522	-0.219682	-0.072997
32	6	0	1.384231	-0.609925	1.950621
33	8	0	0.452256	0.259860	1.726759

34	8	0	1.699511	-1.289285	0.925792
35	6	0	1.971621	-0.798804	3.303591
36	1	0	2.954048	-1.265594	3.216812
37	1	0	2.047736	0.162896	3.815166
38	1	0	1.314162	-1.452843	3.888171
39	8	0	1.731016	1.019469	-0.761470
40	16	0	3.039874	1.612973	-0.225169
41	8	0	4.074404	1.621532	-1.262883
42	8	0	3.404583	1.154768	1.120997
43	6	0	2.539284	3.393612	-0.003534
44	9	0	2.123734	3.907780	-1.171023
45	9	0	1.536830	3.482589	0.880678
46	9	0	3.576897	4.105469	0.440127

SCF Done: E(RB3LYP) = -2595.74194866 A.U. after 1 cycles
Zero-point correction= 0.306495 (Hartree/Particle)
Thermal correction to Energy= 0.336610
Thermal correction to Enthalpy= 0.337554
Thermal correction to Gibbs Free Energy= 0.241444
Sum of electronic and zero-point Energies= -2595.435454
Sum of electronic and thermal Energies= -2595.405339
Sum of electronic and thermal Enthalpies= -2595.404395
Sum of electronic and thermal Free Energies= -2595.500505
SCF Done: E(RB3LYP) = -2597.04241321 A.U. after 26 cycles

SET2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.579019	-1.680906	-2.047486
2	6	0	-2.468368	-1.361770	-1.269384
3	6	0	-2.420883	-1.753907	0.078934
4	6	0	-3.492729	-2.473986	0.635036
5	6	0	-4.603136	-2.781358	-0.143516
6	6	0	-4.647026	-2.385305	-1.484915
7	6	0	-1.251405	-1.483027	0.938398
8	8	0	-1.068917	-1.982254	2.035686
9	7	0	-0.286953	-0.533916	0.437171

10	6	0	1.014709	-0.851287	0.350921
11	6	0	1.874025	0.249612	-0.021516
12	6	0	1.608692	-2.123517	0.542174
13	6	0	3.264257	0.094048	-0.205644
14	6	0	2.979851	-2.288330	0.366996
15	6	0	1.958051	2.518983	-0.530217
16	6	0	4.001217	1.243707	-0.575200
17	6	0	3.800371	-1.220117	0.002085
18	6	0	3.345381	2.449246	-0.738142
19	7	0	1.251693	1.444671	-0.181866
20	17	0	5.496568	-1.496763	-0.201888
21	8	0	-1.217647	3.202615	0.022709
22	6	0	-2.412740	2.843401	0.330715
23	8	0	-2.568544	1.592094	0.548076
24	6	0	-3.528941	3.826599	0.455969
25	1	0	-3.611650	-1.382411	-3.090781
26	1	0	-1.637259	-0.821212	-1.712077
27	1	0	-3.439508	-2.777964	1.675009
28	1	0	-5.433821	-3.329518	0.290348
29	1	0	-5.513817	-2.628754	-2.092527
30	1	0	0.999545	-2.970278	0.832354
31	1	0	3.422945	-3.266249	0.515589
32	1	0	1.406592	3.445986	-0.641896
33	1	0	5.072101	1.174507	-0.728003
34	1	0	3.885870	3.344503	-1.021892
35	1	0	-3.510278	4.256023	1.464793
36	1	0	-3.397474	4.639315	-0.262055
37	1	0	-4.490036	3.330923	0.306756
38	27	0	-0.657816	1.356394	0.190605

SCF Done: E(UB3LYP) = -1634.14691425 A.U. after 1 cycles

Zero-point correction= 0.276838 (Hartree/Particle)

Thermal correction to Energy= 0.298619

Thermal correction to Enthalpy= 0.299563

Thermal correction to Gibbs Free Energy= 0.222748

Sum of electronic and zero-point Energies= -1633.870077

Sum of electronic and thermal Energies= -1633.848296

Sum of electronic and thermal Enthalpies= -1633.847351

Sum of electronic and thermal Free Energies= -1633.924166

SCF Done: E(UB3LYP) = -1635.22298667 A.U. after 31 cycles

SET3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.236809	4.055041	-2.457894
2	6	0	1.339966	2.990065	-1.567471
3	6	0	1.669510	3.228376	-0.222319
4	6	0	1.907063	4.542618	0.220063
5	6	0	1.801174	5.602020	-0.673407
6	6	0	1.464772	5.359590	-2.010719
7	6	0	1.798339	2.136685	0.752641
8	8	0	2.176023	2.243642	1.902438
9	7	0	1.418921	0.804840	0.276526
10	6	0	2.288848	-0.210373	0.282556
11	6	0	1.729159	-1.474019	-0.134060
12	6	0	3.671701	-0.158097	0.602219
13	6	0	2.508511	-2.641374	-0.248261
14	6	0	4.448004	-1.303755	0.503457
15	6	0	-0.202967	-2.569513	-0.834825
16	6	0	1.855420	-3.816296	-0.685497
17	6	0	3.899971	-2.524524	0.088883
18	6	0	0.505538	-3.771957	-0.981512
19	7	0	0.403849	-1.456712	-0.420238
20	17	0	4.922724	-3.903919	-0.014865
21	1	0	0.981684	3.869499	-3.496406
22	1	0	1.174699	1.974922	-1.913504
23	1	0	2.165601	4.712738	1.259692
24	1	0	1.977772	6.617284	-0.332434
25	1	0	1.382082	6.190045	-2.705664
26	1	0	4.120834	0.771617	0.928272
27	1	0	5.501995	-1.257965	0.751389
28	1	0	-1.260655	-2.495892	-1.050128
29	1	0	2.411590	-4.740955	-0.787342
30	1	0	-0.020703	-4.655262	-1.322829
31	27	0	-0.396345	0.273428	-0.011802
32	6	0	-1.209780	1.268268	1.883135
33	8	0	-0.812951	0.040393	1.804674

34	8	0	-1.063282	1.901781	0.783393
35	6	0	-1.727088	1.869067	3.134920
36	1	0	-2.513688	2.587188	2.894462
37	1	0	-2.103778	1.090514	3.800264
38	1	0	-0.906619	2.399816	3.632377
39	8	0	-2.047861	-0.254654	-0.786942
40	16	0	-3.538880	-0.000753	-0.430647
41	8	0	-4.265886	0.470473	-1.607457
42	8	0	-3.725842	0.681270	0.852341
43	6	0	-4.079696	-1.761895	-0.139577
44	9	0	-3.814546	-2.507628	-1.219884
45	9	0	-3.414842	-2.265202	0.905593
46	9	0	-5.386862	-1.792406	0.108513

SCF Done: E(UB3LYP) = -2595.53100291 A.U. after 1 cycles
Zero-point correction= 0.306463 (Hartree/Particle)
Thermal correction to Energy= 0.336636
Thermal correction to Enthalpy= 0.337580
Thermal correction to Gibbs Free Energy= 0.241465
Sum of electronic and zero-point Energies= -2595.224540
Sum of electronic and thermal Energies= -2595.194367
Sum of electronic and thermal Enthalpies= -2595.193423
Sum of electronic and thermal Free Energies= -2595.289538
SCF Done: E(UB3LYP) = -2596.82460511 A.U. after 35 cycles

OTf^-

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.909181	-0.000143	0.000114
2	8	0	1.244057	1.132925	0.895134
3	8	0	1.244118	-1.341730	0.533983
4	8	0	1.246070	0.208480	-1.428282
5	6	0	-0.949727	-0.000036	-0.000147
6	9	0	-1.433660	1.161728	-0.477035
7	9	0	-1.434656	-0.993526	-0.767787
8	9	0	-1.434183	-0.167636	1.243976

SCF Done: E(RB3LYP) = -961.577953096   A.U. after   1 cycles
Zero-point correction=   0.027166 (Hartree/Particle)
 Thermal correction to Energy=   0.034333
 Thermal correction to Enthalpy=   0.035277
 Thermal correction to Gibbs Free Energy=   -0.005342
 Sum of electronic and zero-point Energies=   -961.550787
 Sum of electronic and thermal Energies=   -961.543620
 Sum of electronic and thermal Enthalpies=   -961.542676
 Sum of electronic and thermal Free Energies=   -961.583295
SCF Done: E(RB3LYP) = -961.814091946   A.U. after   12 cycles

Ag_2CO_3

                        Standard orientation:

 Center   Atomic   Atomic   Coordinates (Angstroms)
 Number   Number   Type   X   Y   Z
 ----
      1   6   0   0.211609   2.075893   0.000252
      2   8   0   1.309699   1.340753   -0.002630
      3   47   0   1.398479   -0.781270   0.000382
      4   8   0   0.303618   3.322615   -0.000928
      5   47   0   -1.532159   -0.535487   -0.000519
      6   8   0   -0.986653   1.515664   0.004180

SCF Done: E(RB3LYP) = -555.369679273   A.U. after   1 cycles
Zero-point correction=   0.015545 (Hartree/Particle)
 Thermal correction to Energy=   0.021988
 Thermal correction to Enthalpy=   0.022932
 Thermal correction to Gibbs Free Energy=   -0.019463
 Sum of electronic and zero-point Energies=   -555.354134
 Sum of electronic and thermal Energies=   -555.347692
 Sum of electronic and thermal Enthalpies=   -555.346747
 Sum of electronic and thermal Free Energies=   -555.389142
SCF Done: E(RB3LYP) = -557.937556816   A.U. after   14 cycles

$Ag_2CO_3^{\cdot -}$

                        Standard orientation:

 Center   Atomic   Atomic   Coordinates (Angstroms)
 Number   Number   Type   X   Y   Z

1	6	0	2.082479	0.597036	-0.000021
2	8	0	1.800424	-0.694228	-0.000450
3	47	0	-0.266043	-1.486954	0.000065
4	8	0	3.285878	0.966744	0.000024
5	47	0	-1.057073	1.107751	-0.000062
6	8	0	1.125144	1.507524	0.000427

SCF Done: E(UB3LYP) = -555.487612568 A.U. after 1 cycles
Zero-point correction= 0.015470 (Hartree/Particle)
Thermal correction to Energy= 0.022744
Thermal correction to Enthalpy= 0.023689
Thermal correction to Gibbs Free Energy= -0.021395
Sum of electronic and zero-point Energies= -555.472143
Sum of electronic and thermal Energies= -555.464868
Sum of electronic and thermal Enthalpies= -555.463924
Sum of electronic and thermal Free Energies= -555.509007
SCF Done: E(UB3LYP) = -558.066190062 A.U. after 18 cycles

Scheme 8
Int4_S

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-3.236347	3.563746	-0.989246
2	1	0	-0.761371	3.151680	-0.996922
3	6	0	4.930617	-2.033252	-0.169717
4	6	0	2.550254	-1.687304	-0.048393
5	6	0	2.712186	-0.316569	-0.306503
6	6	0	3.995939	0.192290	-0.499030
7	6	0	5.101104	-0.670356	-0.432781
8	1	0	5.795274	-2.689166	-0.117125
9	1	0	4.152628	1.248409	-0.701910
10	1	0	6.101798	-0.272436	-0.584918
11	6	0	1.145116	-2.155688	0.109908
12	8	0	0.814013	-3.319096	0.346297
13	7	0	0.277597	-1.092856	-0.081165
14	6	0	-1.753354	0.109865	-0.207192

15	6	0	-3.170257	0.251755	-0.163838
16	6	0	-2.851190	2.576437	-0.760215
17	6	0	-1.460741	2.353045	-0.771015
18	7	0	-0.935282	1.166259	-0.501240
19	6	0	3.647222	-2.548882	0.021501
20	1	0	3.485409	-3.605835	0.216586
21	6	0	-1.103345	-1.141593	0.043660
22	6	0	-1.901258	-2.238257	0.356316
23	1	0	-1.439444	-3.196052	0.548224
24	6	0	-3.305663	-2.108491	0.413834
25	1	0	-3.903618	-2.979598	0.660474
26	6	0	-3.699404	1.534204	-0.453046
27	1	0	-4.773089	1.685584	-0.432562
28	6	0	-3.928933	-0.906324	0.161078
29	17	0	-5.685872	-0.807943	0.240871
30	8	0	1.786826	2.442470	-0.522706
31	6	0	1.768051	2.484551	0.747950
32	8	0	1.330203	1.417961	1.319283
33	6	0	2.241126	3.656411	1.546025
34	1	0	3.296418	3.506438	1.802718
35	1	0	2.152800	4.571302	0.956728
36	1	0	1.672274	3.740561	2.474620
37	27	0	1.028434	0.594623	-0.352922

SCF Done: E(RB3LYP) = -1633.69700537 A.U. after 1 cycles

Zero-point correction= 0.265823 (Hartree/Particle)

Thermal correction to Energy= 0.286634

Thermal correction to Enthalpy= 0.287578

Thermal correction to Gibbs Free Energy= 0.215680

Sum of electronic and zero-point Energies= -1633.431183

Sum of electronic and thermal Energies= -1633.410371

Sum of electronic and thermal Enthalpies= -1633.409427

Sum of electronic and thermal Free Energies= -1633.481325

SCF Done: E(RB3LYP) = -1634.77826906 A.U. after 26 cycles

Int4_T

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	1	0	-3.124754	3.677922	-0.709147
2	1	0	-0.663629	3.178357	-0.695631
3	6	0	4.814031	-2.280844	-0.179428
4	6	0	2.450517	-1.855211	-0.024668
5	6	0	2.676819	-0.484277	-0.198839
6	6	0	3.971594	-0.003591	-0.378169
7	6	0	5.039223	-0.912032	-0.367887
8	1	0	5.653215	-2.970676	-0.171482
9	1	0	4.162792	1.053153	-0.536471
10	1	0	6.053612	-0.547060	-0.508183
11	6	0	1.028665	-2.267953	0.114458
12	8	0	0.642121	-3.424554	0.276191
13	7	0	0.215990	-1.146608	0.019363
14	6	0	-1.777357	0.129264	-0.121971
15	6	0	-3.189147	0.316345	-0.114257
16	6	0	-2.777870	2.665132	-0.538408
17	6	0	-1.396862	2.396201	-0.529238
18	7	0	-0.919353	1.176560	-0.322875
19	6	0	3.514871	-2.759923	-0.009544
20	1	0	3.313381	-3.818916	0.127797
21	6	0	-1.176066	-1.154770	0.069216
22	6	0	-2.017753	-2.242573	0.273137
23	1	0	-1.594165	-3.225675	0.418290
24	6	0	-3.419798	-2.071444	0.290697
25	1	0	-4.051622	-2.937898	0.454638
26	6	0	-3.667450	1.632285	-0.328644
27	1	0	-4.735910	1.818092	-0.329541
28	6	0	-3.995948	-0.835294	0.103691
29	17	0	-5.748849	-0.682798	0.133741
30	8	0	1.806854	2.311110	-0.705246
31	6	0	2.005315	2.663884	0.517051
32	8	0	1.693806	1.856399	1.434854
33	6	0	2.626778	4.003835	0.812647
34	1	0	3.717600	3.907669	0.754417
35	1	0	2.314426	4.745469	0.073797
36	1	0	2.363487	4.333335	1.819568
37	27	0	1.031330	0.540974	-0.193797

SCF Done: E(UB3LYP) = -1633.70984591 A.U. after 1 cycles

Zero-point correction= 0.264573 (Hartree/Particle)
Thermal correction to Energy= 0.286072
Thermal correction to Enthalpy= 0.287017
Thermal correction to Gibbs Free Energy= 0.211796
Sum of electronic and zero-point Energies= -1633.445273
Sum of electronic and thermal Energies= -1633.423773
Sum of electronic and thermal Enthalpies= -1633.422829
Sum of electronic and thermal Free Energies= -1633.498050
SCF Done: E(UB3LYP) = -1634.79653044 A.U. after 50 cycles

AcOH

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.091846	0.122699	-0.000043
2	8	0	-0.643841	1.204203	-0.000118
3	8	0	-0.779320	-1.043527	0.000094
4	1	0	-1.728361	-0.813628	0.000145
5	6	0	1.396398	-0.111345	0.000012
6	1	0	1.683382	-0.691555	0.883007
7	1	0	1.683280	-0.693251	-0.881886
8	1	0	1.919672	0.844905	-0.000886

SCF Done: E(RB3LYP) = -229.087580450 A.U. after 1 cycles
Zero-point correction= 0.061820 (Hartree/Particle)
Thermal correction to Energy= 0.066404
Thermal correction to Enthalpy= 0.067349
Thermal correction to Gibbs Free Energy= 0.034489
Sum of electronic and zero-point Energies= -229.025760
Sum of electronic and thermal Energies= -229.021176
Sum of electronic and thermal Enthalpies= -229.020232
Sum of electronic and thermal Free Energies= -229.053091
SCF Done: E(RB3LYP) = -229.171348366 A.U. after 11 cycles

TfOH

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	16	0	0.851798	-0.143546	-0.061536
2	8	0	1.218738	-1.277518	0.767232
3	8	0	1.254173	-0.024406	-1.456392
4	8	0	1.273683	1.189665	0.756204
5	1	0	1.455329	1.920815	0.130148
6	6	0	-1.012233	0.012582	0.001921
7	9	0	-1.414047	0.021657	1.268217
8	9	0	-1.379155	1.141767	-0.599661
9	9	0	-1.538292	-1.030257	-0.634495

SCF Done: E(RB3LYP) = -962.006742463 A.U. after 1 cycles
Zero-point correction= 0.038298 (Hartree/Particle)
Thermal correction to Energy= 0.046155
Thermal correction to Enthalpy= 0.047099
Thermal correction to Gibbs Free Energy= 0.004964
Sum of electronic and zero-point Energies= -961.968444
Sum of electronic and thermal Energies= -961.960588
Sum of electronic and thermal Enthalpies= -961.959644
Sum of electronic and thermal Free Energies= -962.001779
SCF Done: E(RB3LYP) = -962.224551389 A.U. after 13 cycles

I_2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	53	0	0.000000	-0.000000	1.432886
2	53	0	0.000000	-0.000000	-1.432886

SCF Done: E(RB3LYP) = -22.7710623633 A.U. after 1 cycles
Zero-point correction= 0.000412 (Hartree/Particle)
Thermal correction to Energy= 0.003364
Thermal correction to Enthalpy= 0.004308
Thermal correction to Gibbs Free Energy= -0.025550
Sum of electronic and zero-point Energies= -22.770650
Sum of electronic and thermal Energies= -22.767699
Sum of electronic and thermal Enthalpies= -22.766754

Sum of electronic and thermal Free Energies= -22.796612

SCF Done: E(RB3LYP) = -22.8359062499 A.U. after 6 cycles

Int4-I_2_S

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-3.256273	-1.743906	-3.609500
2	1	0	-1.140764	-0.455576	-3.213847
3	6	0	2.749617	4.119431	1.717226
4	6	0	0.904879	2.590165	1.480485
5	6	0	1.237729	2.353508	0.136594
6	6	0	2.338793	3.006054	-0.413881
7	6	0	3.091997	3.882280	0.380436
8	1	0	3.341616	4.804318	2.317339
9	1	0	2.623035	2.841280	-1.449261
10	1	0	3.953991	4.386454	-0.049982
11	6	0	-0.257465	1.848452	2.011729
12	8	0	-0.754373	1.979630	3.120972
13	7	0	-0.745414	0.942910	1.020588
14	6	0	-2.413984	-0.227329	-0.187377
15	6	0	-3.645830	-0.926600	-0.320159
16	6	0	-3.052782	-1.325838	-2.630247
17	6	0	-1.860181	-0.608464	-2.415864
18	7	0	-1.556994	-0.077442	-1.239943
19	6	0	1.650513	3.470367	2.274829
20	1	0	1.365020	3.629533	3.311053
21	6	0	-2.002883	0.344304	1.060357
22	6	0	-2.851351	0.223804	2.157454
23	1	0	-2.560895	0.643374	3.109549
24	6	0	-4.085327	-0.443476	2.031928
25	1	0	-4.734270	-0.519487	2.897271
26	6	0	-3.944648	-1.478413	-1.590482
27	1	0	-4.873011	-2.019598	-1.734831
28	6	0	-4.474340	-1.009957	0.835752
29	17	0	-6.012015	-1.845237	0.745500
30	8	0	0.614920	1.507237	-2.560829
31	6	0	-0.206326	2.480962	-2.595315

32	8	0	-0.882173	2.658263	-1.517273
33	6	0	-0.362718	3.381711	-3.777106
34	1	0	0.342716	4.215462	-3.679563
35	1	0	-0.131264	2.839319	-4.696236
36	1	0	-1.374824	3.789975	-3.815482
37	27	0	-0.008241	1.164413	-0.708606
38	53	0	1.183064	-0.961037	0.717282
39	53	0	3.274812	-2.959460	-0.239419

SCF Done: E(RB3LYP) = -1656.47967928 A.U. after 1 cycles
Zero-point correction= 0.266842 (Hartree/Particle)
Thermal correction to Energy= 0.292322
Thermal correction to Enthalpy= 0.293266
Thermal correction to Gibbs Free Energy= 0.206516
Sum of electronic and zero-point Energies= -1656.212837
Sum of electronic and thermal Energies= -1656.187357
Sum of electronic and thermal Enthalpies= -1656.186413
Sum of electronic and thermal Free Energies= -1656.273163
SCF Done: E(RB3LYP) = -1657.62554352 A.U. after 27 cycles

Int4-I_2_T

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	3.238682	0.295032	3.327199
2	1	0	0.861325	-0.399258	2.932009
3	6	0	-5.415579	0.426316	-1.600050
4	6	0	-3.096930	1.011090	-1.316428
5	6	0	-3.011769	0.226278	-0.149753
6	6	0	-4.145337	-0.461533	0.285929
7	6	0	-5.337637	-0.358547	-0.438632
8	1	0	-6.350284	0.492113	-2.148818
9	1	0	-4.106934	-1.078897	1.178288
10	1	0	-6.218322	-0.897530	-0.097980
11	6	0	-1.874274	1.709300	-1.733653
12	8	0	-1.732485	2.427025	-2.712858
13	7	0	-0.828695	1.431262	-0.794364
14	6	0	1.244404	1.524390	0.301039

15	6	0	2.581359	1.969480	0.434690
16	6	0	2.703226	0.663559	2.460004
17	6	0	1.372360	0.268596	2.247022
18	7	0	0.668109	0.690142	1.200313
19	6	0	-4.293077	1.114513	-2.044193
20	1	0	-4.322263	1.727569	-2.940514
21	6	0	0.411538	1.940094	-0.813367
22	6	0	0.972262	2.817344	-1.780087
23	1	0	0.366243	3.136506	-2.615314
24	6	0	2.285238	3.255543	-1.649289
25	1	0	2.701347	3.923843	-2.394485
26	6	0	3.310916	1.512888	1.555935
27	1	0	4.338090	1.828255	1.698160
28	6	0	3.081799	2.851721	-0.577359
29	17	0	4.709462	3.438804	-0.480413
30	8	0	-1.842802	-0.423443	2.414906
31	6	0	-2.130723	0.762724	2.788585
32	8	0	-1.926753	1.677856	1.914851
33	6	0	-2.697585	1.069826	4.137941
34	1	0	-3.786746	0.949430	4.098776
35	1	0	-2.303040	0.372064	4.880105
36	1	0	-2.472847	2.100018	4.421522
37	27	0	-1.287356	0.324445	0.671239
38	53	0	-0.677307	-1.959790	-0.605331
39	53	0	2.604322	-2.904203	-0.351693

SCF Done: E(UB3LYP) = -1656.48802327 A.U. after 1 cycles

Zero-point correction= 0.266441 (Hartree/Particle)

Thermal correction to Energy= 0.292139

Thermal correction to Enthalpy= 0.293083

Thermal correction to Gibbs Free Energy= 0.203765

Sum of electronic and zero-point Energies= -1656.221582

Sum of electronic and thermal Energies= -1656.195884

Sum of electronic and thermal Enthalpies= -1656.194940

Sum of electronic and thermal Free Energies= -1656.284258

SCF Done: E(UB3LYP) = -1657.63072571 A.U. after 51 cycles

TSOA1_T

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.825761	-3.795613	1.282987
2	1	0	0.554740	-2.756146	1.115459
3	6	0	-3.378416	3.894014	-0.219474
4	6	0	-1.221071	2.832809	-0.276953
5	6	0	-1.769310	1.619679	0.175829
6	6	0	-3.136714	1.552889	0.444278
7	6	0	-3.930680	2.686848	0.240530
8	1	0	-4.015840	4.760568	-0.367631
9	1	0	-3.583445	0.636076	0.811641
10	1	0	-4.997039	2.632805	0.445976
11	6	0	0.219984	2.840813	-0.524176
12	8	0	0.904696	3.770538	-0.921140
13	7	0	0.763491	1.541531	-0.223710
14	6	0	2.334601	-0.163948	0.184784
15	6	0	3.659647	-0.662171	0.243910
16	6	0	2.725590	-2.763703	0.966965
17	6	0	1.447377	-2.187942	0.878385
18	7	0	1.259958	-0.927862	0.494015
19	6	0	-2.016981	3.973110	-0.478693
20	1	0	-1.557690	4.892202	-0.831218
21	6	0	2.061086	1.205117	-0.213018
22	6	0	3.160463	2.043936	-0.544665
23	1	0	2.971724	3.064884	-0.841006
24	6	0	4.458682	1.552933	-0.487977
25	1	0	5.287182	2.203777	-0.743173
26	6	0	3.834124	-2.005278	0.647792
27	1	0	4.830291	-2.428368	0.705987
28	6	0	4.718685	0.236617	-0.105996
29	17	0	6.363007	-0.305997	-0.054048
30	8	0	-1.943965	-0.166145	2.873766
31	6	0	-0.927518	0.499165	3.063974
32	8	0	-0.078401	0.831831	2.122640
33	6	0	-0.538239	1.035375	4.433467
34	1	0	-0.682953	2.121465	4.454915
35	1	0	-1.161559	0.575954	5.203078
36	1	0	0.517749	0.839084	4.641552
37	27	0	-0.455630	0.256411	0.375583

38	53	0	-0.876306	-0.615253	-2.208399
39	53	0	-2.374424	-2.467669	0.129748

SCF Done: E(UB3LYP) = -1656.45357686 A.U. after 1 cycles
Zero-point correction= 0.265357 (Hartree/Particle)
Thermal correction to Energy= 0.290778
Thermal correction to Enthalpy= 0.291722
Thermal correction to Gibbs Free Energy= 0.204262
Sum of electronic and zero-point Energies= -1656.188219
Sum of electronic and thermal Energies= -1656.162799
Sum of electronic and thermal Enthalpies= -1656.161855
Sum of electronic and thermal Free Energies= -1656.249315
SCF Done: E(UB3LYP) = -1657.59945226 A.U. after 124 cycles

Int5_T

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	3.100835	-3.843107	-0.305697
2	1	0	0.755888	-3.001352	-0.263629
3	6	0	-3.724737	3.484650	0.738671
4	6	0	-1.506690	2.573960	0.502563
5	6	0	-2.005260	1.267033	0.325240
6	6	0	-3.392580	1.094200	0.358731
7	6	0	-4.236879	2.190869	0.563667
8	1	0	-4.396738	4.323146	0.895641
9	1	0	-3.836135	0.115155	0.221202
10	1	0	-5.312604	2.033163	0.585831
11	6	0	-0.055304	2.748136	0.458576
12	8	0	0.559919	3.799896	0.571103
13	7	0	0.576658	1.477767	0.269662
14	6	0	2.288223	-0.130006	0.128087
15	6	0	3.654450	-0.511999	0.113798
16	6	0	2.911987	-2.783101	-0.180653
17	6	0	1.588187	-2.315383	-0.156547
18	7	0	1.281878	-1.028808	-0.005800
19	6	0	-2.351449	3.678101	0.706572
20	1	0	-1.912866	4.663654	0.834214

21	6	0	1.898925	1.259218	0.279346
22	6	0	2.924682	2.234417	0.417002
23	1	0	2.648862	3.272013	0.528724
24	6	0	4.262416	1.857376	0.408715
25	1	0	5.031430	2.613685	0.517317
26	6	0	3.949709	-1.884241	-0.045306
27	1	0	4.980436	-2.218819	-0.061153
28	6	0	4.633279	0.522740	0.261735
29	17	0	6.321369	0.120937	0.260513
30	8	0	-1.778289	-1.971920	2.535832
31	6	0	-1.029221	-1.009534	2.840258
32	8	0	-0.464186	-0.178884	2.052712
33	6	0	-0.762874	-0.780402	4.322716
34	1	0	-1.297591	0.121952	4.637919
35	1	0	-1.105846	-1.629910	4.914448
36	1	0	0.306014	-0.614219	4.481472
37	27	0	-0.578408	-0.023756	0.131462
38	53	0	-0.650338	0.238622	-2.553053
39	53	0	-2.078689	-2.211481	-0.095018

SCF Done: E(UB3LYP) = -1656.46357868 A.U. after 1 cycles
Zero-point correction= 0.265782 (Hartree/Particle)
Thermal correction to Energy= 0.291636
Thermal correction to Enthalpy= 0.292580
Thermal correction to Gibbs Free Energy= 0.204748
Sum of electronic and zero-point Energies= -1656.197797
Sum of electronic and thermal Energies= -1656.171943
Sum of electronic and thermal Enthalpies= -1656.170999
Sum of electronic and thermal Free Energies= -1656.258831
SCF Done: E(UB3LYP) = -1657.60945531 A.U. after 53 cycles

TSOA2_T

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	3.164112	-3.655164	-1.262110
2	1	0	0.823375	-2.852899	-0.972220
3	6	0	-3.711757	2.895820	1.487790

4	6	0	-1.466544	2.359504	0.775033
5	6	0	-1.971954	1.248211	0.056573
6	6	0	-3.360969	1.013582	-0.001875
7	6	0	-4.216334	1.817300	0.746406
8	1	0	-4.392178	3.533042	2.044512
9	1	0	-3.761381	0.210470	-0.607691
10	1	0	-5.283550	1.617224	0.733761
11	6	0	0.011066	2.542769	0.858706
12	8	0	0.543501	3.585741	1.254550
13	7	0	0.632883	1.400022	0.458867
14	6	0	2.380459	-0.114603	-0.012511
15	6	0	3.750824	-0.488240	-0.143447
16	6	0	2.984122	-2.647371	-0.905016
17	6	0	1.657757	-2.200648	-0.744808
18	7	0	1.362825	-0.983903	-0.308808
19	6	0	-2.339745	3.161211	1.505055
20	1	0	-1.927524	3.975887	2.092788
21	6	0	1.998279	1.188814	0.428918
22	6	0	3.001038	2.099509	0.752515
23	1	0	2.731063	3.089584	1.089999
24	6	0	4.358130	1.737728	0.633956
25	1	0	5.121330	2.464825	0.890341
26	6	0	4.025116	-1.799781	-0.603199
27	1	0	5.053813	-2.123598	-0.715450
28	6	0	4.729320	0.485024	0.197992
29	17	0	6.440350	0.088647	0.067040
30	8	0	-1.668775	-2.358224	2.301001
31	6	0	-0.912173	-1.432291	2.709311
32	8	0	-0.361797	-0.520208	2.018307
33	53	0	-1.059279	0.973400	-2.307132
34	6	0	-0.623486	-1.405727	4.204230
35	1	0	-0.934758	-0.437417	4.607702
36	1	0	-1.146827	-2.210822	4.720976
37	1	0	0.455670	-1.505033	4.357077
38	27	0	-0.465815	-0.109300	0.103770
39	53	0	-1.971747	-2.331856	-0.301099

SCF Done: E(UB3LYP) = -1656.44376655 A.U. after 1 cycles

Zero-point correction= 0.264595 (Hartree/Particle)

Thermal correction to Energy= 0.290052

Thermal correction to Enthalpy= 0.290996
Thermal correction to Gibbs Free Energy= 0.204543
Sum of electronic and zero-point Energies= -1656.179171
Sum of electronic and thermal Energies= -1656.153715
Sum of electronic and thermal Enthalpies= -1656.152771
Sum of electronic and thermal Free Energies= -1656.239224
SCF Done: E(UB3LYP) = -1657.59310248 A.U. after 52 cycles

Int6_T

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-4.048611	3.252842	-1.185124
2	1	0	-1.581837	3.178174	-0.805005
3	6	0	4.241978	-2.582319	1.287916
4	6	0	1.910823	-1.990701	0.858892
5	6	0	2.171988	-2.068765	-0.518478
6	6	0	3.448639	-2.384827	-0.986926
7	6	0	4.484999	-2.628061	-0.085546
8	1	0	5.039650	-2.783261	1.996127
9	1	0	3.635490	-2.451639	-2.052490
10	1	0	5.475130	-2.864275	-0.464032
11	6	0	0.604479	-1.679545	1.519692
12	8	0	0.295913	-2.209178	2.577100
13	7	0	-0.243951	-0.709743	0.924383
14	6	0	-2.330375	0.171236	0.298254
15	6	0	-3.735066	0.115589	0.104433
16	6	0	-3.597789	2.360700	-0.766165
17	6	0	-2.208908	2.332376	-0.552487
18	7	0	-1.593065	1.269040	-0.039819
19	6	0	2.967372	-2.276877	1.745716
20	1	0	2.759326	-2.236315	2.809373
21	6	0	-1.598629	-0.921585	0.860554
22	6	0	-2.303242	-2.080319	1.211931
23	1	0	-1.784667	-2.925956	1.642739
24	6	0	-3.691506	-2.150867	1.027096
25	1	0	-4.219271	-3.053886	1.312254
26	6	0	-4.361279	1.258384	-0.445421

27	1	0	-5.433131	1.260754	-0.607426
28	6	0	-4.397512	-1.087930	0.491217
29	17	0	-6.126874	-1.226137	0.296028
30	8	0	0.385451	1.969861	2.482569
31	6	0	1.576521	1.552165	2.479647
32	8	0	1.984563	0.891261	1.449859
33	6	0	2.536437	1.824341	3.603827
34	1	0	3.169702	2.676690	3.330714
35	1	0	1.991971	2.069743	4.517529
36	1	0	3.186697	0.961260	3.766709
37	27	0	0.298478	1.061138	0.505927
38	53	0	0.663509	-1.866638	-2.041293
39	53	0	1.319993	2.987409	-1.053555

SCF Done: E(UB3LYP) = -1656.49758892 A.U. after 1 cycles

Zero-point correction= 0.265632 (Hartree/Particle)

Thermal correction to Energy= 0.291637

Thermal correction to Enthalpy= 0.292582

Thermal correction to Gibbs Free Energy= 0.203531

Sum of electronic and zero-point Energies= -1656.231957

Sum of electronic and thermal Energies= -1656.205951

Sum of electronic and thermal Enthalpies= -1656.205007

Sum of electronic and thermal Free Energies= -1656.294058

SCF Done: E(UB3LYP) = -1657.64349648 A.U. after 43 cycles

Int7_D

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-3.420830	-3.613348	0.025237
2	1	0	-0.948312	-3.186703	-0.045917
3	6	0	4.637924	2.200257	-0.739620
4	6	0	2.266184	1.824520	-0.557790
5	6	0	2.461231	0.434314	-0.439174
6	6	0	3.764272	-0.064978	-0.478341
7	6	0	4.841035	0.814864	-0.627331
8	1	0	5.488136	2.866570	-0.851886
9	1	0	3.948477	-1.131241	-0.387434

10	1	0	5.854110	0.420333	-0.653873
11	6	0	0.879294	2.300432	-0.514368
12	8	0	0.492389	3.458446	-0.590545
13	7	0	-0.000770	1.177193	-0.377057
14	6	0	-1.978713	-0.080157	-0.262630
15	6	0	-3.388139	-0.216123	-0.225303
16	6	0	-3.046916	-2.599282	-0.056889
17	6	0	-1.661507	-2.370873	-0.097530
18	7	0	-1.148478	-1.148284	-0.198481
19	6	0	3.346796	2.710314	-0.705764
20	1	0	3.156277	3.776595	-0.789959
21	6	0	-1.342132	1.219849	-0.364247
22	6	0	-2.172123	2.369315	-0.433578
23	1	0	-1.714019	3.344491	-0.509530
24	6	0	-3.557191	2.236991	-0.400371
25	1	0	-4.179182	3.123354	-0.452854
26	6	0	-3.912869	-1.524580	-0.120339
27	1	0	-4.985667	-1.676309	-0.089124
28	6	0	-4.163257	0.985954	-0.298459
29	17	0	-5.896458	0.897429	-0.260553
30	8	0	1.578887	-2.315662	-0.684153
31	6	0	1.397327	-2.093295	-1.927963
32	8	0	0.882407	-0.959532	-2.222330
33	27	0	0.816599	-0.523616	-0.304415
34	53	0	0.994780	-0.512276	2.368593
35	6	0	1.790410	-3.080369	-2.983408
36	1	0	2.855476	-2.951098	-3.209577
37	1	0	1.641370	-4.100156	-2.620548
38	1	0	1.217954	-2.911800	-3.897723

SCF Done: E(UB3LYP) = -1645.10460749 A.U. after 1 cycles

Zero-point correction= 0.266096 (Hartree/Particle)

Thermal correction to Energy= 0.289179

Thermal correction to Enthalpy= 0.290123

Thermal correction to Gibbs Free Energy= 0.211275

Sum of electronic and zero-point Energies= -1644.838512

Sum of electronic and thermal Energies= -1644.815429

Sum of electronic and thermal Enthalpies= -1644.814485

Sum of electronic and thermal Free Energies= -1644.893333

SCF Done: E(UB3LYP) = -1646.21502306 A.U. after 50 cycles

TSHD_D

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	3.405583	3.587881	0.891697
2	1	0	0.950674	3.134653	0.610150
3	6	0	-4.435984	-1.686437	-1.517150
4	6	0	-2.131257	-1.633148	-0.789618
5	6	0	-2.398620	-0.417456	-0.110884
6	6	0	-3.693179	0.134789	-0.098143
7	6	0	-4.696585	-0.487787	-0.835797
8	1	0	-5.234875	-2.179109	-2.063198
9	1	0	-3.898236	1.039944	0.461951
10	1	0	-5.690708	-0.051620	-0.864321
11	6	0	-0.712514	-2.109414	-0.877777
12	8	0	-0.400040	-3.261716	-1.196910
13	7	0	0.117466	-1.069936	-0.592655
14	6	0	2.090258	0.140005	-0.162943
15	6	0	3.498843	0.302773	-0.032173
16	6	0	3.068718	2.601858	0.591861
17	6	0	1.689069	2.358534	0.439066
18	7	0	1.224366	1.173053	0.074089
19	6	0	-3.156399	-2.249989	-1.502369
20	1	0	-2.931736	-3.154285	-2.060255
21	6	0	1.498981	-1.105684	-0.542925
22	6	0	2.342039	-2.182705	-0.797975
23	1	0	1.918926	-3.134348	-1.087821
24	6	0	3.740037	-2.034662	-0.675465
25	1	0	4.379046	-2.887661	-0.878412
26	6	0	3.966658	1.583195	0.357613
27	1	0	5.032129	1.751459	0.469661
28	6	0	4.307918	-0.834446	-0.305045
29	17	0	6.059979	-0.711625	-0.171632
30	8	0	-1.425760	2.447126	-0.238911
31	6	0	-1.311916	2.488002	-1.515236
32	8	0	-0.829537	1.451699	-2.078041
33	27	0	-0.681937	0.616401	-0.242520

34	53	0	-1.443457	-0.221430	2.212156
35	6	0	-1.755867	3.686301	-2.299868
36	1	0	-2.845363	3.651195	-2.417761
37	1	0	-1.505285	4.603519	-1.760707
38	1	0	-1.295567	3.687857	-3.289634

SCF Done: E(UB3LYP) = -1645.08541903 A.U. after 1 cycles
Zero-point correction= 0.264593 (Hartree/Particle)
Thermal correction to Energy= 0.287485
Thermal correction to Enthalpy= 0.288429
Thermal correction to Gibbs Free Energy= 0.209795
Sum of electronic and zero-point Energies= -1644.820826
Sum of electronic and thermal Energies= -1644.797934
Sum of electronic and thermal Enthalpies= -1644.796990
Sum of electronic and thermal Free Energies= -1644.875624
SCF Done: E(UB3LYP) = -1646.20029824 A.U. after 48 cycles

Int8_D

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	4.368580	3.267098	1.420413
2	1	0	1.895951	3.376885	0.974953
3	6	0	-4.129708	-0.387946	-2.485864
4	6	0	-2.097915	-0.901183	-1.240295
5	6	0	-2.873914	-1.002694	-0.083540
6	6	0	-4.254085	-0.799853	-0.107198
7	6	0	-4.881124	-0.484899	-1.313371
8	1	0	-4.613296	-0.153002	-3.429565
9	1	0	-4.838704	-0.889974	0.801750
10	1	0	-5.955555	-0.325731	-1.331325
11	6	0	-0.628692	-1.255594	-1.321162
12	8	0	-0.353537	-2.341576	-1.843868
13	7	0	0.275367	-0.349943	-0.832488
14	6	0	2.457079	0.333174	-0.170599
15	6	0	3.858501	0.185999	0.039267
16	6	0	3.860795	2.422056	0.969618
17	6	0	2.477019	2.495294	0.727734

18	7	0	1.813196	1.484859	0.179803
19	6	0	-2.755736	-0.606896	-2.445524
20	1	0	-2.168919	-0.554741	-3.358575
21	6	0	1.638884	-0.687090	-0.746549
22	6	0	2.280051	-1.866422	-1.119055
23	1	0	1.711682	-2.665741	-1.566600
24	6	0	3.669276	-2.033793	-0.920832
25	1	0	4.129695	-2.968756	-1.222612
26	6	0	4.546269	1.276258	0.626964
27	1	0	5.613413	1.199392	0.803497
28	6	0	4.443814	-1.045651	-0.359565
29	17	0	6.170419	-1.310079	-0.138286
30	8	0	-0.493113	3.289768	0.336639
31	6	0	-1.707071	3.121377	-0.065883
32	8	0	-1.985176	1.989500	-0.564712
33	27	0	-0.060948	1.474191	-0.238704
34	53	0	-1.993224	-1.522750	1.818050
35	6	0	-2.714195	4.224067	0.054061
36	1	0	-2.766803	4.561170	1.094200
37	1	0	-2.391091	5.077354	-0.552074
38	1	0	-3.696486	3.886805	-0.279767

SCF Done: E(UB3LYP) = -1645.10845075 A.U. after 1 cycles
Zero-point correction= 0.265381 (Hartree/Particle)
Thermal correction to Energy= 0.289126
Thermal correction to Enthalpy= 0.290070
Thermal correction to Gibbs Free Energy= 0.207051
Sum of electronic and zero-point Energies= -1644.843069
Sum of electronic and thermal Energies= -1644.819325
Sum of electronic and thermal Enthalpies= -1644.818381
Sum of electronic and thermal Free Energies= -1644.901400
SCF Done: E(UB3LYP) = -1646.22558937 A.U. after 66 cycles

TSEC_T

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-3.529385	1.082231	3.739773

2	1	0	-1.485851	-0.279347	3.210406
3	6	0	2.188429	-4.294936	-1.841927
4	6	0	0.853722	-2.283794	-1.760987
5	6	0	1.509003	-1.890112	-0.564040
6	6	0	2.499391	-2.727835	-0.021251
7	6	0	2.818245	-3.932858	-0.645302
8	1	0	2.457652	-5.223371	-2.336003
9	1	0	3.023674	-2.429412	0.880625
10	1	0	3.572574	-4.581969	-0.211036
11	6	0	-0.344072	-1.531255	-2.230667
12	8	0	-0.750781	-1.501417	-3.381007
13	7	0	-0.990996	-0.949540	-1.124468
14	6	0	-2.591423	0.167424	0.144994
15	6	0	-3.759021	0.941441	0.342260
16	6	0	-3.293901	0.838702	2.710372
17	6	0	-2.148525	0.074939	2.428993
18	7	0	-1.815558	-0.252357	1.182806
19	6	0	1.200394	-3.478680	-2.394412
20	1	0	0.668451	-3.774965	-3.293151
21	6	0	-2.142202	-0.219248	-1.161453
22	6	0	-2.892937	0.184199	-2.278122
23	1	0	-2.574102	-0.097410	-3.271665
24	6	0	-4.052845	0.947795	-2.097556
25	1	0	-4.625676	1.255299	-2.964941
26	6	0	-4.100000	1.271075	1.674542
27	1	0	-4.986231	1.862187	1.875522
28	6	0	-4.484155	1.320926	-0.831350
29	17	0	-5.933241	2.269211	-0.678107
30	8	0	0.372697	-1.734839	2.339947
31	6	0	-0.184345	-2.900959	2.351776
32	8	0	-0.839554	-3.256605	1.336223
33	6	0	-0.042768	-3.767362	3.573293
34	1	0	1.010080	-3.835321	3.863076
35	1	0	-0.584966	-3.309850	4.408391
36	1	0	-0.444773	-4.763930	3.384413
37	27	0	-0.255088	-1.279481	0.556963
38	53	0	1.981651	0.387045	-0.197362
39	53	0	2.894577	3.539458	0.198112

SCF Done: E(UB3LYP) = -1656.47668315 A.U. after 1 cycles

Zero-point correction= 0.264761 (Hartree/Particle)
Thermal correction to Energy= 0.290345
Thermal correction to Enthalpy= 0.291289
Thermal correction to Gibbs Free Energy= 0.202866
Sum of electronic and zero-point Energies= -1656.211923
Sum of electronic and thermal Energies= -1656.186339
Sum of electronic and thermal Enthalpies= -1656.185394
Sum of electronic and thermal Free Energies= -1656.273817
SCF Done: E(UB3LYP) = -1657.62226413 A.U. after 55 cycles

Int9_T

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	4.182273	-0.767535	2.725035
2	1	0	1.687384	-0.947606	2.947996
3	6	0	-5.129004	1.918839	-1.380673
4	6	0	-2.754891	1.696855	-0.844573
5	6	0	-2.835819	0.321811	-1.139967
6	6	0	-4.046873	-0.236539	-1.550937
7	6	0	-5.190807	0.554120	-1.666465
8	1	0	-6.013527	2.541952	-1.466989
9	1	0	-4.103439	-1.294450	-1.782864
10	1	0	-6.125190	0.098520	-1.981225
11	6	0	-1.547230	2.470288	-0.434757
12	8	0	-1.491476	3.686738	-0.543515
13	7	0	-0.454177	1.771043	0.155845
14	6	0	1.809281	1.369656	0.616813
15	6	0	3.197302	1.538544	0.416747
16	6	0	3.538434	-0.144229	2.116039
17	6	0	2.144685	-0.254696	2.250967
18	7	0	1.314489	0.487953	1.522226
19	6	0	-3.922017	2.477153	-0.984230
20	1	0	-3.850920	3.536543	-0.764706
21	6	0	0.823960	2.101407	-0.139129
22	6	0	1.283548	3.005045	-1.125328
23	1	0	0.576762	3.566676	-1.720516
24	6	0	2.650513	3.188678	-1.326375

25	1	0	2.987721	3.889396	-2.081503
26	6	0	4.067309	0.750008	1.205494
27	1	0	5.140327	0.844897	1.085519
28	6	0	3.594847	2.486028	-0.581001
29	17	0	5.279300	2.761380	-0.883008
30	8	0	-0.973734	-0.721649	3.071160
31	6	0	-2.225757	-0.453500	2.967756
32	8	0	-2.536805	0.381158	2.051276
33	6	0	-3.246891	-1.107296	3.840420
34	1	0	-3.498439	-2.086635	3.416131
35	1	0	-2.839857	-1.266663	4.841751
36	1	0	-4.154121	-0.501852	3.884840
37	27	0	-0.621456	0.485650	1.594618
38	53	0	-1.175221	-1.073885	-1.044669
39	53	0	1.623761	-3.460930	-0.822684

SCF Done: E(UB3LYP) = -1656.49135398 A.U. after 1 cycles
Zero-point correction= 0.265769 (Hartree/Particle)
Thermal correction to Energy= 0.291931
Thermal correction to Enthalpy= 0.292875
Thermal correction to Gibbs Free Energy= 0.201204
Sum of electronic and zero-point Energies= -1656.225584
Sum of electronic and thermal Energies= -1656.199423
Sum of electronic and thermal Enthalpies= -1656.198479
Sum of electronic and thermal Free Energies= -1656.290150
SCF Done: E(UB3LYP) = -1657.63534170 A.U. after 49 cycles

Scheme S1
TSOA1_S

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	3.018718	-3.697150	1.326918
2	1	0	0.687466	-2.809531	1.133882
3	6	0	-3.612019	3.650934	0.065830
4	6	0	-1.427689	2.672044	-0.167767
5	6	0	-1.897388	1.434212	0.308314
6	6	0	-3.235345	1.318109	0.687789

7	6	0	-4.083693	2.423586	0.558871
8	1	0	-4.288984	4.495241	-0.025466
9	1	0	-3.617854	0.386899	1.090195
10	1	0	-5.126971	2.331077	0.850973
11	6	0	-0.001183	2.739879	-0.509515
12	8	0	0.612787	3.715915	-0.920534
13	7	0	0.610255	1.476966	-0.256004
14	6	0	2.300164	-0.112945	0.179780
15	6	0	3.657603	-0.527709	0.250177
16	6	0	2.855049	-2.677772	0.996755
17	6	0	1.541068	-2.186120	0.892132
18	7	0	1.275261	-0.947280	0.491690
19	6	0	-2.276443	3.781328	-0.295867
20	1	0	-1.878485	4.720149	-0.670467
21	6	0	1.942543	1.222978	-0.238353
22	6	0	2.978533	2.116621	-0.584230
23	1	0	2.728286	3.118019	-0.901373
24	6	0	4.311088	1.712317	-0.509737
25	1	0	5.094768	2.414492	-0.770876
26	6	0	3.912375	-1.854548	0.673701
27	1	0	4.933499	-2.211803	0.741696
28	6	0	4.654739	0.426526	-0.107457
29	17	0	6.337214	-0.008486	-0.038660
30	8	0	-1.794565	-0.581955	2.990069
31	6	0	-0.866785	0.212667	3.132941
32	8	0	-0.134744	0.686490	2.154411
33	6	0	-0.461268	0.765154	4.492456
34	1	0	-0.749187	1.820561	4.558116
35	1	0	-0.963255	0.207463	5.285544
36	1	0	0.623195	0.710816	4.626415
37	27	0	-0.511220	0.130224	0.402425
38	53	0	-0.808753	-0.473865	-2.248902
39	53	0	-2.187576	-2.390908	-0.050156

SCF Done: E(RB3LYP) = -1656.43412968 A.U. after 1 cycles

Zero-point correction= 0.265381 (Hartree/Particle)

Thermal correction to Energy= 0.290721

Thermal correction to Enthalpy= 0.291665

Thermal correction to Gibbs Free Energy= 0.205805

Sum of electronic and zero-point Energies= -1656.168749

Sum of electronic and thermal Energies= -1656.143408

Sum of electronic and thermal Enthalpies= -1656.142464

Sum of electronic and thermal Free Energies= -1656.228325

SCF Done: E(RB3LYP) = -1657.58279187 A.U. after 31 cycles

Int5_S

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	3.155975	-3.822511	0.914918
2	1	0	0.770316	-3.072417	0.806394
3	6	0	-3.971286	3.228407	-0.019665
4	6	0	-1.720044	2.381118	-0.118636
5	6	0	-2.145561	1.071830	0.178010
6	6	0	-3.508309	0.864287	0.395214
7	6	0	-4.407023	1.934146	0.295118
8	1	0	-4.684658	4.043440	-0.095938
9	1	0	-3.885457	-0.123048	0.633481
10	1	0	-5.465643	1.752185	0.464447
11	6	0	-0.290855	2.589318	-0.314583
12	8	0	0.291945	3.605990	-0.626660
13	7	0	0.420700	1.311564	-0.071727
14	6	0	2.196661	-0.199466	0.160041
15	6	0	3.576783	-0.526104	0.182449
16	6	0	2.925546	-2.786550	0.695287
17	6	0	1.583329	-2.374056	0.640266
18	7	0	1.227879	-1.116543	0.374756
19	6	0	-2.617743	3.456236	-0.227263
20	1	0	-2.238760	4.445763	-0.466159
21	6	0	1.752322	1.149610	-0.115728
22	6	0	2.725361	2.152211	-0.369110
23	1	0	2.403331	3.163097	-0.570187
24	6	0	4.074398	1.834041	-0.348212
25	1	0	4.812359	2.604420	-0.538121
26	6	0	3.928037	-1.867398	0.462605
27	1	0	4.970574	-2.162222	0.491898
28	6	0	4.502034	0.529406	-0.080192
29	17	0	6.196597	0.211950	-0.067941

30	8	0	0.263951	2.028977	2.239393
31	6	0	-0.235452	1.024110	2.779211
32	8	0	-0.678153	-0.021150	2.165643
33	6	0	-0.387093	0.978901	4.292664
34	1	0	0.269357	1.712467	4.763398
35	1	0	-1.426701	1.217204	4.544274
36	1	0	-0.169055	-0.025066	4.664935
37	27	0	-0.669875	-0.168607	0.279135
38	53	0	-0.643860	-0.326708	-2.425599
39	53	0	-2.077193	-2.460086	0.439409

SCF Done: E(RB3LYP) = -1656.45008071 A.U. after 1 cycles
Zero-point correction= 0.265994 (Hartree/Particle)
Thermal correction to Energy= 0.291736
Thermal correction to Enthalpy= 0.292680
Thermal correction to Gibbs Free Energy= 0.207252
Sum of electronic and zero-point Energies= -1656.184087
Sum of electronic and thermal Energies= -1656.158345
Sum of electronic and thermal Enthalpies= -1656.157401
Sum of electronic and thermal Free Energies= -1656.242829
SCF Done: E(RB3LYP) = -1657.59284284 A.U. after 27 cycles

TSOA2_S

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	3.054255	-3.828232	-0.631167
2	1	0	0.706770	-3.025768	-0.324668
3	6	0	-3.864281	3.124314	0.751388
4	6	0	-1.601438	2.416344	0.353038
5	6	0	-2.054862	1.086621	0.060327
6	6	0	-3.456521	0.840711	0.026173
7	6	0	-4.335356	1.834827	0.417333
8	1	0	-4.575423	3.899758	1.019416
9	1	0	-3.823524	-0.136744	-0.261143
10	1	0	-5.401153	1.630019	0.449762
11	6	0	-0.150896	2.653291	0.348150
12	8	0	0.397935	3.745359	0.468663

13	7	0	0.502262	1.427210	0.177805
14	6	0	2.229688	-0.130627	-0.089461
15	6	0	3.588163	-0.481938	-0.296706
16	6	0	2.862237	-2.771715	-0.484498
17	6	0	1.538879	-2.331484	-0.304052
18	7	0	1.236448	-1.053216	-0.090814
19	6	0	-2.501962	3.416495	0.713515
20	1	0	-2.127325	4.403766	0.964586
21	6	0	1.832312	1.243929	0.110685
22	6	0	2.835965	2.242632	0.150175
23	1	0	2.549172	3.270332	0.318618
24	6	0	4.169636	1.896423	-0.032706
25	1	0	4.932588	2.665774	0.000749
26	6	0	3.888221	-1.852051	-0.488416
27	1	0	4.914593	-2.165449	-0.640646
28	6	0	4.548006	0.571391	-0.253773
29	17	0	6.234455	0.213410	-0.442234
30	8	0	1.582497	-0.247612	2.669935
31	6	0	0.386561	-0.158559	2.948486
32	8	0	-0.615706	-0.085423	2.113542
33	53	0	-1.223880	0.246214	-2.373770
34	6	0	-0.089779	-0.128846	4.400647
35	1	0	-0.708585	-1.009357	4.603668
36	1	0	0.769787	-0.123126	5.073749
37	1	0	-0.708479	0.755713	4.581152
38	27	0	-0.578265	-0.152377	0.222740
39	53	0	-2.021242	-2.446168	0.368902

SCF Done: E(RB3LYP) = -1656.43571429   A.U. after   1 cycles

Zero-point correction=   0.264825 (Hartree/Particle)

Thermal correction to Energy=   0.290138

Thermal correction to Enthalpy=   0.291082

Thermal correction to Gibbs Free Energy=   0.206330

Sum of electronic and zero-point Energies=   -1656.170889

Sum of electronic and thermal Energies=   -1656.145577

Sum of electronic and thermal Enthalpies=   -1656.144632

Sum of electronic and thermal Free Energies=   -1656.229384

SCF Done: E(RB3LYP) = -1657.58239502   A.U. after   30 cycles

Int6_S

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-3.773108	2.742115	-2.242864
2	1	0	-1.356912	2.677963	-1.630471
3	6	0	4.237585	-1.846488	1.834960
4	6	0	1.942605	-1.792941	1.010932
5	6	0	2.443452	-1.838479	-0.295687
6	6	0	3.817429	-1.865009	-0.545827
7	6	0	4.714155	-1.853521	0.522394
8	1	0	4.930572	-1.858366	2.670781
9	1	0	4.187724	-1.907008	-1.564031
10	1	0	5.781683	-1.868108	0.322923
11	6	0	0.481519	-1.836461	1.382949
12	8	0	0.079272	-2.797136	2.042842
13	7	0	-0.329711	-0.822106	0.922954
14	6	0	-2.355417	0.039923	0.086207
15	6	0	-3.754310	0.028288	-0.177893
16	6	0	-3.410894	1.966975	-1.577576
17	6	0	-2.045002	1.935308	-1.248346
18	7	0	-1.538495	1.006210	-0.442831
19	6	0	2.867540	-1.829202	2.069088
20	1	0	2.485930	-1.830501	3.085524
21	6	0	-1.720484	-0.947772	0.893794
22	6	0	-2.526761	-1.920596	1.478342
23	1	0	-2.081906	-2.681469	2.100362
24	6	0	-3.918767	-1.935831	1.245658
25	1	0	-4.519402	-2.709482	1.711622
26	6	0	-4.264119	1.030494	-1.036592
27	1	0	-5.324063	1.052549	-1.263677
28	6	0	-4.521918	-0.998824	0.438181
29	17	0	-6.256109	-1.073908	0.169108
30	8	0	-0.293838	1.769858	1.973452
31	6	0	0.880661	1.595649	2.484574
32	8	0	1.689714	1.001173	1.710756
33	6	0	1.224017	2.095082	3.845275
34	1	0	1.424497	3.171204	3.788031
35	1	0	0.383218	1.940686	4.526121

36	1	0	2.115958	1.585984	4.214359
37	27	0	0.216956	0.932985	0.387833
38	53	0	1.158393	-2.032097	-2.021719
39	53	0	1.350482	3.003999	-0.859505

SCF Done: E(RB3LYP) = -1656.48624090 A.U. after 1 cycles
Zero-point correction= 0.267283 (Hartree/Particle)
Thermal correction to Energy= 0.292599
Thermal correction to Enthalpy= 0.293543
Thermal correction to Gibbs Free Energy= 0.208564
Sum of electronic and zero-point Energies= -1656.218957
Sum of electronic and thermal Energies= -1656.193642
Sum of electronic and thermal Enthalpies= -1656.192698
Sum of electronic and thermal Free Energies= -1656.277677
SCF Done: E(RB3LYP) = -1657.63194166 A.U. after 27 cycles

Int9_S

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-4.050332	1.848066	1.910336
2	1	0	-1.546860	1.761652	2.081271
3	6	0	4.826368	-2.684296	-1.085508
4	6	0	2.494012	-2.143414	-0.601022
5	6	0	2.772401	-0.814245	-0.951360
6	6	0	4.043519	-0.415634	-1.360084
7	6	0	5.073899	-1.354313	-1.428551
8	1	0	5.623700	-3.419603	-1.129275
9	1	0	4.239436	0.618426	-1.623904
10	1	0	6.063628	-1.039794	-1.745931
11	6	0	1.160205	-2.727954	-0.228098
12	8	0	0.960395	-3.929315	-0.393834
13	7	0	0.174359	-1.888333	0.293425
14	6	0	-2.034115	-1.091955	0.493979
15	6	0	-3.441796	-1.109900	0.316777
16	6	0	-3.509998	1.004133	1.498429
17	6	0	-2.109729	0.966330	1.607902
18	7	0	-1.411841	-0.057436	1.125743

19	6	0	3.551641	-3.068252	-0.686206
20	1	0	3.339172	-4.100287	-0.430465
21	6	0	-1.175383	-2.125466	0.025515
22	6	0	-1.764709	-3.190685	-0.655564
23	1	0	-1.157918	-4.007150	-1.017916
24	6	0	-3.160102	-3.230010	-0.847249
25	1	0	-3.592125	-4.075659	-1.370703
26	6	0	-4.171434	-0.020428	0.850446
27	1	0	-5.250001	0.005278	0.742285
28	6	0	-3.985318	-2.229052	-0.374874
29	17	0	-5.713545	-2.348349	-0.618298
30	8	0	0.901216	1.050734	2.614364
31	6	0	2.049358	0.506096	2.764211
32	8	0	2.273801	-0.500645	2.001835
33	6	0	3.065852	1.018710	3.729341
34	1	0	3.695662	1.756654	3.218212
35	1	0	2.573452	1.509249	4.571435
36	1	0	3.703566	0.202844	4.076030
37	27	0	0.469863	-0.319001	1.291325
38	53	0	1.289389	0.783772	-0.906797
39	53	0	-0.831396	3.638709	-0.899951

SCF Done: E(RB3LYP) = -1656.46732683 A.U. after 1 cycles
Zero-point correction= 0.266980 (Hartree/Particle)
Thermal correction to Energy= 0.292539
Thermal correction to Enthalpy= 0.293483
Thermal correction to Gibbs Free Energy= 0.206314
Sum of electronic and zero-point Energies= -1656.200347
Sum of electronic and thermal Energies= -1656.174788
Sum of electronic and thermal Enthalpies= -1656.173843
Sum of electronic and thermal Free Energies= -1656.261013
SCF Done: E(RB3LYP) = -1657.61568242 A.U. after 29 cycles

Scheme S5
Int1_OAc_S

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-3.249189	-3.644695	1.471101
2	6	0	-2.054383	-3.096353	1.002042
3	6	0	-1.706173	-3.211448	-0.349005
4	6	0	-2.569162	-3.897615	-1.218609
5	6	0	-3.771051	-4.427508	-0.754667
6	6	0	-4.113846	-4.304886	0.595580
7	6	0	-0.380719	-2.766331	-0.898939
8	8	0	0.101126	-3.423616	-1.832535
9	7	0	0.291019	-1.702130	-0.315677
10	6	0	1.670028	-1.584208	-0.497454
11	6	0	2.233502	-0.343065	-0.076441
12	6	0	2.567057	-2.556178	-0.945951
13	6	0	3.635439	-0.080036	-0.083543
14	6	0	3.954904	-2.315371	-0.966586
15	6	0	1.768745	1.765714	0.819158
16	6	0	4.062748	1.184301	0.392557
17	6	0	4.484861	-1.113737	-0.553418
18	6	0	3.137211	2.096355	0.844994
19	7	0	1.351019	0.596215	0.364296
20	17	0	6.230091	-0.864091	-0.612975
21	1	0	-3.505335	-3.553645	2.523513
22	1	0	-1.398497	-2.562368	1.675280
23	1	0	-2.281713	-4.010998	-2.258977
24	1	0	-4.437066	-4.942308	-1.442206
25	1	0	-5.046786	-4.725142	0.962233
26	1	0	2.201217	-3.512325	-1.285745
27	1	0	4.616066	-3.100096	-1.319708
28	1	0	1.008288	2.452118	1.163405
29	1	0	5.121330	1.419492	0.402381
30	1	0	3.439869	3.067101	1.221322
31	27	0	-0.473781	0.022001	0.168949
32	6	0	-1.888589	0.029545	-1.681720
33	8	0	-0.675648	0.429562	-1.749503
34	8	0	-2.265862	-0.401879	-0.541733
35	6	0	-2.791850	0.007440	-2.873693
36	1	0	-3.778145	0.382770	-2.592596
37	1	0	-2.374558	0.612597	-3.680217
38	1	0	-2.903184	-1.027506	-3.216989
39	8	0	-1.134613	1.893744	0.681418
40	16	0	-2.011833	2.986704	0.106415

41	8	0	-2.718530	3.721265	1.166533
42	8	0	-2.790690	2.615886	-1.085382
43	6	0	-0.748843	4.200515	-0.528016
44	9	0	0.022676	4.643067	0.480228
45	9	0	0.044758	3.629729	-1.444830
46	9	0	-1.361361	5.251815	-1.086126
47	6	0	0.090048	-0.724699	2.904191
48	8	0	-0.767898	-0.372016	1.981026
49	8	0	1.285515	-0.970095	2.755429
50	6	0	-0.574787	-0.818084	4.278444
51	1	0	-1.398066	-1.540091	4.254434
52	1	0	0.156956	-1.123720	5.029203
53	1	0	-1.002333	0.151541	4.554986

SCF Done: E(RB3LYP) = -2824.40453636 A.U. after 1 cycles
Zero-point correction= 0.357565 (Hartree/Particle)
Thermal correction to Energy= 0.393042
Thermal correction to Enthalpy= 0.393986
Thermal correction to Gibbs Free Energy= 0.286335
Sum of electronic and zero-point Energies= -2824.046971
Sum of electronic and thermal Energies= -2824.011494
Sum of electronic and thermal Enthalpies= -2824.010550
Sum of electronic and thermal Free Energies= -2824.118201
SCF Done: E(RB3LYP) = -2825.79122128 A.U. after 18 cycles

Int2_OAc_S

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.023188	2.605549	-0.467413
2	6	0	1.725103	2.218380	-0.815980
3	6	0	0.659277	3.127741	-0.707971
4	6	0	0.910407	4.436197	-0.282639
5	6	0	2.206579	4.820284	0.062007
6	6	0	3.263051	3.905161	-0.021332
7	6	0	-0.754131	2.700296	-0.957102
8	8	0	-1.615918	3.493431	-1.357640
9	7	0	-0.988609	1.392937	-0.637101

10	6	0	-2.243243	0.808890	-0.591492
11	6	0	-2.267525	-0.410515	0.144607
12	6	0	-3.439656	1.253756	-1.144042
13	6	0	-3.448924	-1.173832	0.344993
14	6	0	-4.623597	0.503146	-0.970910
15	6	0	-0.978599	-1.909406	1.405443
16	6	0	-3.333963	-2.346846	1.132749
17	6	0	-4.637941	-0.671802	-0.251102
18	6	0	-2.113553	-2.704877	1.662951
19	7	0	-1.078577	-0.810219	0.679362
20	17	0	-6.150474	-1.555149	-0.058144
21	1	0	3.835640	1.893001	-0.568647
22	1	0	1.581608	1.284830	-1.373525
23	1	0	0.083302	5.135548	-0.210708
24	1	0	2.395428	5.835593	0.400235
25	1	0	4.269883	4.212506	0.247248
26	1	0	-3.463316	2.179754	-1.699007
27	1	0	-5.544177	0.867500	-1.414805
28	1	0	0.008822	-2.168887	1.765916
29	1	0	-4.212586	-2.955931	1.314482
30	1	0	-2.004070	-3.596618	2.269530
31	27	0	0.346609	0.290761	0.114720
32	6	0	0.568955	-0.597048	-2.673095
33	8	0	0.367068	-0.866611	-1.414659
34	8	0	0.846762	0.503783	-3.155443
35	6	0	0.447234	-1.836427	-3.556621
36	1	0	0.600184	-1.570573	-4.604471
37	1	0	1.193082	-2.576558	-3.250567
38	1	0	-0.539714	-2.294584	-3.432692
39	8	0	1.777754	-0.861545	0.945302
40	16	0	3.111734	-1.342425	0.401861
41	8	0	4.148193	-1.334033	1.446093
42	8	0	3.474258	-0.794135	-0.914221
43	6	0	2.789309	-3.157300	0.116523
44	9	0	2.285286	-3.711134	1.232072
45	9	0	1.923571	-3.359034	-0.882247
46	9	0	3.939244	-3.775467	-0.185115
47	6	0	-0.438943	1.730138	2.498164
48	8	0	0.499055	1.282577	1.704796
49	8	0	-1.647579	1.522008	2.404850

50	6	0	0.135394	2.592837	3.621445
51	1	0	0.608612	3.484638	3.196068
52	1	0	-0.658837	2.894381	4.307576
53	1	0	0.908121	2.043154	4.168678

SCF Done: E(RB3LYP) = -2824.38925169 A.U. after 1 cycles
Zero-point correction= 0.357147 (Hartree/Particle)
Thermal correction to Energy= 0.392728
Thermal correction to Enthalpy= 0.393672
Thermal correction to Gibbs Free Energy= 0.287463
Sum of electronic and zero-point Energies= -2824.032105
Sum of electronic and thermal Energies= -2823.996524
Sum of electronic and thermal Enthalpies= -2823.995579
Sum of electronic and thermal Free Energies= -2824.101788
SCF Done: E(RB3LYP) = -2825.77830030 A.U. after 17 cycles

TS2-3_OAc_S

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.847010	2.379769	-0.139065
2	6	0	1.521276	2.075240	-0.497776
3	6	0	0.593686	3.140849	-0.578848
4	6	0	0.974718	4.460793	-0.345583
5	6	0	2.298973	4.735906	0.004565
6	6	0	3.233405	3.698317	0.109132
7	6	0	-0.830156	2.781408	-0.849545
8	8	0	-1.688875	3.598307	-1.209283
9	7	0	-1.040663	1.452433	-0.608903
10	6	0	-2.273223	0.826082	-0.596915
11	6	0	-2.274783	-0.434136	0.076927
12	6	0	-3.470337	1.274039	-1.145481
13	6	0	-3.448647	-1.227378	0.209750
14	6	0	-4.641142	0.492776	-1.034406
15	6	0	-0.992119	-1.968665	1.278471
16	6	0	-3.328235	-2.442309	0.931077
17	6	0	-4.638317	-0.719372	-0.380125
18	6	0	-2.112258	-2.805614	1.465919

19	7	0	-1.084530	-0.833111	0.610976
20	17	0	-6.135801	-1.647018	-0.267764
21	1	0	3.584587	1.583718	-0.097762
22	1	0	1.516120	1.329867	-1.580329
23	1	0	0.235100	5.253062	-0.417592
24	1	0	2.605605	5.760927	0.196530
25	1	0	4.262631	3.923612	0.376563
26	1	0	-3.503608	2.229765	-1.648300
27	1	0	-5.562505	0.860894	-1.473853
28	1	0	-0.011452	-2.228240	1.658552
29	1	0	-4.198993	-3.076160	1.058764
30	1	0	-1.998093	-3.728461	2.023817
31	27	0	0.363304	0.415947	0.104982
32	6	0	0.989695	-0.340240	-2.595638
33	8	0	0.414480	-0.682014	-1.518786
34	8	0	1.570780	0.775804	-2.759155
35	6	0	0.985604	-1.336971	-3.730613
36	1	0	1.428523	-0.907592	-4.630099
37	1	0	1.559116	-2.215802	-3.419056
38	1	0	-0.038676	-1.662857	-3.934006
39	8	0	1.804742	-0.795376	0.913726
40	16	0	3.099335	-1.398503	0.419741
41	8	0	4.101147	-1.498524	1.493973
42	8	0	3.561739	-0.891901	-0.883576
43	6	0	2.628205	-3.173170	0.094205
44	9	0	2.061179	-3.712719	1.187166
45	9	0	1.761813	-3.276256	-0.922637
46	9	0	3.723568	-3.882974	-0.209099
47	6	0	-0.571366	1.634933	2.570788
48	8	0	0.413423	1.259637	1.803576
49	8	0	-1.778026	1.540665	2.344092
50	6	0	-0.062599	2.256125	3.874409
51	1	0	0.521772	3.155991	3.654126
52	1	0	-0.903551	2.518132	4.520295
53	1	0	0.599173	1.557135	4.396582

SCF Done: E(RB3LYP) = -2824.37546696 A.U. after 1 cycles

Zero-point correction= 0.352654 (Hartree/Particle)

Thermal correction to Energy= 0.387409

Thermal correction to Enthalpy= 0.388353

Thermal correction to Gibbs Free Energy= 0.285473
Sum of electronic and zero-point Energies= -2824.022813
Sum of electronic and thermal Energies= -2823.988058
Sum of electronic and thermal Enthalpies= -2823.987114
Sum of electronic and thermal Free Energies= -2824.089994
SCF Done: E(RB3LYP) = -2825.76458953 A.U. after 17 cycles

Int3_OAc_S

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.855444	2.230071	0.288170
2	6	0	1.495601	2.032748	0.023222
3	6	0	0.738252	3.131194	-0.428076
4	6	0	1.312389	4.389748	-0.623595
5	6	0	2.671287	4.570346	-0.360660
6	6	0	3.437714	3.492625	0.092619
7	6	0	-0.706904	2.868375	-0.679718
8	8	0	-1.496627	3.714668	-1.125376
9	7	0	-1.009005	1.574152	-0.355183
10	6	0	-2.249181	0.980263	-0.466000
11	6	0	-2.311740	-0.366819	0.022860
12	6	0	-3.415006	1.535409	-0.990254
13	6	0	-3.518198	-1.126643	-0.000679
14	6	0	-4.610302	0.787624	-1.031771
15	6	0	-1.136049	-2.102396	1.033147
16	6	0	-3.466549	-2.436934	0.539193
17	6	0	-4.668916	-0.502248	-0.552888
18	6	0	-2.285921	-2.919460	1.057750
19	7	0	-1.155084	-0.881336	0.529877
20	17	0	-6.198657	-1.385431	-0.626415
21	1	0	3.475115	1.413143	0.644089
22	1	0	2.090813	1.397961	-1.810560
23	1	0	0.689209	5.208199	-0.974405
24	1	0	3.132545	5.543330	-0.508078
25	1	0	4.496372	3.631705	0.299614
26	1	0	-3.399022	2.551453	-1.356477
27	1	0	-5.502541	1.245361	-1.446983

28	1	0	-0.185024	-2.449795	1.420168
29	1	0	-4.362713	-3.047940	0.542711
30	1	0	-2.225105	-3.916736	1.480082
31	27	0	0.378691	0.477931	0.309396
32	6	0	1.223738	-0.099965	-2.553288
33	8	0	0.551723	-0.335429	-1.542664
34	8	0	2.043724	0.923343	-2.678235
35	6	0	1.175390	-1.005876	-3.747535
36	1	0	1.500094	-0.487696	-4.651012
37	1	0	1.855467	-1.843348	-3.554372
38	1	0	0.167337	-1.405559	-3.871065
39	8	0	1.791553	-0.874420	0.968834
40	16	0	3.027659	-1.532253	0.407068
41	8	0	4.037534	-1.795421	1.445463
42	8	0	3.511982	-0.962281	-0.863427
43	6	0	2.414998	-3.228979	-0.060706
44	9	0	1.876956	-3.847682	1.004128
45	9	0	1.481660	-3.159051	-1.022143
46	9	0	3.432696	-3.973578	-0.513332
47	6	0	-0.686187	1.339186	2.864226
48	8	0	0.330681	1.020203	2.111583
49	8	0	-1.872045	1.403024	2.542097
50	6	0	-0.240465	1.655705	4.295381
51	1	0	0.427162	2.524397	4.295589
52	1	0	-1.108777	1.865659	4.923879
53	1	0	0.321287	0.813864	4.713760

SCF Done: E(RB3LYP) = -2824.39421275 A.U. after 1 cycles

Zero-point correction= 0.357157 (Hartree/Particle)

Thermal correction to Energy= 0.392915

Thermal correction to Enthalpy= 0.393859

Thermal correction to Gibbs Free Energy= 0.286736

Sum of electronic and zero-point Energies= -2824.037055

Sum of electronic and thermal Energies= -2824.001298

Sum of electronic and thermal Enthalpies= -2824.000354

Sum of electronic and thermal Free Energies= -2824.107477

SCF Done: E(RB3LYP) = -2825.78488249 A.U. after 15 cycles

Int1_OAc_T

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.696120	2.836603	-1.195947
2	6	0	2.346996	2.471872	-1.198312
3	6	0	1.416491	3.233303	-0.479498
4	6	0	1.847332	4.374014	0.216900
5	6	0	3.195849	4.723217	0.230449
6	6	0	4.125697	3.952833	-0.476396
7	6	0	-0.052649	2.938921	-0.473375
8	8	0	-0.854847	3.875703	-0.469771
9	7	0	-0.457761	1.607083	-0.459295
10	6	0	-1.826765	1.299142	-0.481394
11	6	0	-2.249883	0.155890	0.272248
12	6	0	-2.795571	2.003492	-1.184777
13	6	0	-3.624036	-0.222466	0.354987
14	6	0	-4.153830	1.629032	-1.131349
15	6	0	-1.599740	-1.610732	1.637019
16	6	0	-3.939733	-1.347310	1.159678
17	6	0	-4.563318	0.555858	-0.373158
18	6	0	-2.936669	-2.031512	1.806827
19	7	0	-1.282563	-0.562038	0.903432
20	17	0	-6.276907	0.148307	-0.313933
21	1	0	4.410431	2.246476	-1.764044
22	1	0	2.016680	1.620048	-1.788463
23	1	0	1.115946	4.973773	0.749186
24	1	0	3.522357	5.598224	0.786092
25	1	0	5.177001	4.228362	-0.471346
26	1	0	-2.514435	2.862977	-1.775652
27	1	0	-4.883187	2.204135	-1.691691
28	1	0	-0.779309	-2.153570	2.094489
29	1	0	-4.973540	-1.660889	1.254591
30	1	0	-3.154045	-2.893978	2.427384
31	27	0	0.583301	0.139226	0.091223
32	6	0	0.505522	-0.782342	-2.608061
33	8	0	0.009151	-0.892270	-1.402814
34	8	0	1.302559	0.074777	-2.989663
35	6	0	-0.032730	-1.854841	-3.546612
36	1	0	0.425264	-1.758250	-4.533095

37	1	0	0.185686	-2.841501	-3.128128
38	1	0	-1.120623	-1.763710	-3.636768
39	8	0	1.873466	-1.343500	0.597294
40	16	0	2.492940	-2.596139	0.003617
41	8	0	3.656755	-3.024108	0.794947
42	8	0	2.638768	-2.589564	-1.458218
43	6	0	1.213603	-3.906039	0.350384
44	9	0	0.922541	-3.936112	1.662982
45	9	0	0.082426	-3.683057	-0.328358
46	9	0	1.693661	-5.105429	-0.003813
47	6	0	0.716976	1.652447	2.520704
48	8	0	1.332485	0.974486	1.574083
49	8	0	-0.481358	1.905384	2.570143
50	6	0	1.693349	2.130227	3.590850
51	1	0	2.397979	2.842388	3.147973
52	1	0	1.149186	2.613124	4.405078
53	1	0	2.276596	1.289450	3.979096

SCF Done: E(UB3LYP) = -2824.38497113 A.U. after 1 cycles
Zero-point correction= 0.355651 (Hartree/Particle)
Thermal correction to Energy= 0.391888
Thermal correction to Enthalpy= 0.392832
Thermal correction to Gibbs Free Energy= 0.283146
Sum of electronic and zero-point Energies= -2824.029320
Sum of electronic and thermal Energies= -2823.993083
Sum of electronic and thermal Enthalpies= -2823.992139
Sum of electronic and thermal Free Energies= -2824.101825
SCF Done: E(UB3LYP) = -2825.77560449 A.U. after 39 cycles

TS2-3_OAc_T

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.548420	2.653226	-0.117237
2	6	0	1.260438	2.265824	-0.536333
3	6	0	0.237025	3.245756	-0.593995
4	6	0	0.510079	4.581138	-0.309317
5	6	0	1.800834	4.946668	0.082906

6	6	0	2.817907	3.987361	0.182320
7	6	0	-1.160632	2.787243	-0.879336
8	8	0	-2.071053	3.552218	-1.214548
9	7	0	-1.268398	1.441686	-0.646316
10	6	0	-2.454352	0.725672	-0.606011
11	6	0	-2.332186	-0.548264	0.032349
12	6	0	-3.699905	1.092735	-1.100788
13	6	0	-3.433010	-1.439948	0.165988
14	6	0	-4.801961	0.217307	-0.982445
15	6	0	-0.896132	-2.023476	1.139634
16	6	0	-3.196415	-2.667190	0.835309
17	6	0	-4.678640	-1.010894	-0.372244
18	6	0	-1.939772	-2.954799	1.319978
19	7	0	-1.100204	-0.871402	0.526917
20	17	0	-6.089806	-2.060582	-0.250196
21	1	0	3.341882	1.912394	-0.085757
22	1	0	1.339170	1.545106	-1.574760
23	1	0	-0.289006	5.314119	-0.368649
24	1	0	2.016895	5.985353	0.318432
25	1	0	3.817164	4.288305	0.484453
26	1	0	-3.822892	2.055572	-1.576201
27	1	0	-5.763427	0.522751	-1.381777
28	1	0	0.114572	-2.217805	1.480462
29	1	0	-4.010601	-3.372428	0.961131
30	1	0	-1.736125	-3.887510	1.834035
31	27	0	0.261811	0.507507	0.090084
32	6	0	1.119312	-0.254884	-2.643075
33	8	0	0.547083	-0.676989	-1.595617
34	8	0	1.526566	0.936923	-2.803568
35	6	0	1.342236	-1.247542	-3.767191
36	1	0	1.698331	-0.749315	-4.670078
37	1	0	2.086244	-1.978185	-3.433737
38	1	0	0.414571	-1.788251	-3.975415
39	8	0	1.928659	-0.737606	0.836732
40	16	0	3.294814	-1.198815	0.419643
41	8	0	4.255797	-1.238892	1.538073
42	8	0	3.784211	-0.616710	-0.845102
43	6	0	3.007244	-2.998069	0.029948
44	9	0	2.421033	-3.610853	1.074733
45	9	0	2.215966	-3.153542	-1.041020

46	9	0	4.174612	-3.611177	-0.217083
47	6	0	-0.557332	1.386054	2.774233
48	8	0	0.411485	1.227205	1.919889
49	8	0	-1.766095	1.286248	2.544568
50	6	0	-0.054806	1.743016	4.175953
51	1	0	0.562385	2.647011	4.136286
52	1	0	-0.894506	1.902641	4.856326
53	1	0	0.578485	0.935864	4.560878

SCF Done: E(UB3LYP) = -2824.35270645 A.U. after 1 cycles
Zero-point correction= 0.350132 (Hartree/Particle)
Thermal correction to Energy= 0.386140
Thermal correction to Enthalpy= 0.387084
Thermal correction to Gibbs Free Energy= 0.277654
Sum of electronic and zero-point Energies= -2824.002575
Sum of electronic and thermal Energies= -2823.966566
Sum of electronic and thermal Enthalpies= -2823.965622
Sum of electronic and thermal Free Energies= -2824.075053
SCF Done: E(UB3LYP) = -2825.74697755 A.U. after 39 cycles

Int3_OAc_T

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.471732	-1.155952	1.219364
2	6	0	2.221158	-0.554841	1.324803
3	6	0	2.077359	0.671414	1.984040
4	6	0	3.185318	1.309429	2.550363
5	6	0	4.441692	0.713744	2.444226
6	6	0	4.583285	-0.510386	1.779262
7	6	0	0.700010	1.230842	2.029423
8	8	0	0.384304	2.281438	2.596069
9	7	0	-0.159798	0.389654	1.344804
10	6	0	-1.522986	0.598412	1.172768
11	6	0	-2.216048	-0.501913	0.569245
12	6	0	-2.264511	1.725855	1.509984
13	6	0	-3.617789	-0.468845	0.314027
14	6	0	-3.653969	1.771761	1.262555

15	6	0	-2.021369	-2.650808	-0.314920
16	6	0	-4.191663	-1.616080	-0.288200
17	6	0	-4.317084	0.712315	0.685537
18	6	0	-3.399716	-2.699693	-0.602143
19	7	0	-1.459244	-1.593482	0.247718
20	17	0	-6.053792	0.828110	0.401721
21	1	0	3.591949	-2.107679	0.710195
22	1	0	1.160483	2.789908	-1.052718
23	1	0	3.050375	2.259808	3.059963
24	1	0	5.312909	1.199619	2.875218
25	1	0	5.566483	-0.967961	1.696550
26	1	0	-1.769961	2.574402	1.959065
27	1	0	-4.206010	2.665631	1.533469
28	1	0	-1.359737	-3.480398	-0.543782
29	1	0	-5.255301	-1.631274	-0.499624
30	1	0	-3.819898	-3.585519	-1.065468
31	27	0	0.536021	-1.248241	0.672524
32	6	0	0.684934	4.315894	0.008113
33	8	0	-0.466195	4.351681	-0.390104
34	8	0	1.592272	3.428327	-0.427369
35	6	0	1.256681	5.231334	1.063129
36	1	0	1.314990	4.667768	2.000991
37	1	0	2.266661	5.555625	0.797786
38	1	0	0.604307	6.094974	1.201425
39	8	0	0.873945	-0.928007	-1.458712
40	16	0	1.344454	0.230303	-2.289924
41	8	0	2.805015	0.392645	-2.359670
42	8	0	0.560053	1.476082	-2.083497
43	6	0	0.831188	-0.320109	-3.992356
44	9	0	1.441460	-1.468872	-4.313292
45	9	0	-0.493503	-0.508467	-4.049218
46	9	0	1.170379	0.611132	-4.894146
47	6	0	0.905774	-3.538299	1.659864
48	8	0	1.085481	-3.143486	0.444278
49	8	0	0.510999	-2.732520	2.534463
50	6	0	1.199510	-4.987534	1.979809
51	1	0	2.276892	-5.166517	1.888580
52	1	0	0.879451	-5.232379	2.994112
53	1	0	0.697294	-5.642102	1.260833

SCF Done: E(UB3LYP) = -2824.40413009   A.U. after   1 cycles
Zero-point correction=   0.355595 (Hartree/Particle)
 Thermal correction to Energy=   0.392337
 Thermal correction to Enthalpy=   0.393281
 Thermal correction to Gibbs Free Energy=   0.280659
 Sum of electronic and zero-point Energies=   -2824.048535
 Sum of electronic and thermal Energies=   -2824.011793
 Sum of electronic and thermal Enthalpies=   -2824.010849
 Sum of electronic and thermal Free Energies=   -2824.123471
SCF Done: E(UB3LYP) = -2825.80107797   A.U. after   38 cycles

X. Calculated data of spin densities

Scheme 8
Int4_T

Mulliken charges and spin densities:

		1	2
1	H	0.120554	0.001306
2	H	0.127588	-0.001794
3	C	-0.084023	0.024806
4	C	-0.028095	0.029971
5	C	-0.038508	-0.119619
6	C	-0.084670	0.022284
7	C	-0.078500	-0.021000
8	H	0.087101	-0.001234
9	H	0.088052	-0.002607
10	H	0.087231	0.000045
11	C	0.221771	-0.055768
12	O	-0.206305	0.099352
13	N	-0.249474	0.224879
14	C	0.100181	0.032261
15	C	0.012997	-0.035627
16	C	-0.069878	-0.029864
17	C	0.051583	0.041199
18	N	-0.208330	-0.029230
19	C	-0.080028	-0.022843
20	H	0.091512	0.000265
21	C	0.091488	-0.078346

22	C	-0.075880	0.131073
23	H	0.124335	-0.005866
24	C	-0.050161	-0.062580
25	H	0.121599	0.002598
26	C	-0.044885	0.042663
27	H	0.125207	-0.001956
28	C	0.038504	0.108960
29	Cl	-0.195688	0.003235
30	O	-0.204550	0.050025
31	C	0.249445	-0.026933
32	O	-0.169450	0.310565
33	C	-0.251094	0.004724
34	H	0.109569	-0.000675
35	H	0.107666	0.000990
36	H	0.106995	0.000273
37	Co	0.056143	1.364468

Sum of Mulliken charges = -0.00000 2.00000

Int4-I_2_T

Mulliken charges and spin densities:

		1	2
1	H	0.132243	0.002556
2	H	0.138831	-0.003260
3	C	-0.077445	0.028682
4	C	-0.026564	0.031793
5	C	-0.030547	-0.012886
6	C	-0.081760	0.022226
7	C	-0.067400	-0.020736
8	H	0.095961	-0.001308
9	H	0.098652	-0.001222
10	H	0.097074	0.000793
11	C	0.239800	-0.097041
12	O	-0.164408	0.172058
13	N	-0.196649	0.471284
14	C	0.119051	0.113043
15	C	0.021809	-0.091415
16	C	-0.056645	-0.057436
17	C	0.062349	0.071949
18	N	-0.205493	-0.042148

19	C	-0.069314	-0.022784
20	H	0.101140	0.000870
21	C	0.114988	-0.137156
22	C	-0.042889	0.319359
23	H	0.144092	-0.014364
24	C	-0.040850	-0.162746
25	H	0.137900	0.006808
26	C	-0.034003	0.088260
27	H	0.136055	-0.004085
28	C	0.065954	0.329306
29	Cl	-0.139972	0.019122
30	O	-0.173256	-0.011464
31	C	0.269578	-0.000431
32	O	-0.147454	0.019917
33	C	-0.251079	0.000917
34	H	0.122484	0.000012
35	H	0.120438	0.000038
36	H	0.118448	-0.000098
37	Co	0.219831	0.029780
38	I	-0.332404	0.377208
39	I	-0.418544	0.574601

Sum of Mulliken charges = -0.00000 2.00000

TSEC_T

Mulliken charges and spin densities:

		1	2
1	H	0.134112	0.002154
2	H	0.144309	-0.002148
3	C	-0.049580	0.046894
4	C	0.002164	0.052722
5	C	-0.072271	-0.081039
6	C	-0.044356	0.046264
7	C	-0.060957	-0.034881
8	H	0.114697	-0.002206
9	H	0.121239	-0.002740
10	H	0.113914	0.001239
11	C	0.244362	-0.117349
12	O	-0.148651	0.219712
13	N	-0.218597	0.438017

14	C	0.119373	0.092734
15	C	0.023185	-0.074211
16	C	-0.057039	-0.046979
17	C	0.065599	0.054821
18	N	-0.201668	-0.032753
19	C	-0.059086	-0.035425
20	H	0.116588	0.001333
21	C	0.108233	-0.129073
22	C	-0.043282	0.267318
23	H	0.142728	-0.012054
24	C	-0.039061	-0.134875
25	H	0.138390	0.005609
26	C	-0.031674	0.069263
27	H	0.138111	-0.003205
28	C	0.063817	0.260110
29	Cl	-0.144190	0.015128
30	O	-0.197918	-0.054563
31	C	0.257838	-0.011991
32	O	-0.176371	0.197754
33	C	-0.251620	0.004807
34	H	0.112495	0.000060
35	H	0.111601	0.000139
36	H	0.109514	-0.000553
37	Co	0.236080	0.916091
38	I	-0.114177	0.045140
39	I	-0.707849	0.038737

Sum of Mulliken charges = -0.00000 2.00000

Int9_T

Mulliken charges and spin densities:

		1	2
1	H	0.136228	0.002261
2	H	0.149521	-0.002938
3	C	-0.069701	0.007477
4	C	-0.010610	0.013671
5	C	-0.026698	-0.014558
6	C	-0.064693	0.007205
7	C	-0.058813	-0.011082
8	H	0.106434	-0.000303

9	H	0.112629	-0.000419
10	H	0.109163	0.000468
11	C	0.250731	-0.080197
12	O	-0.150644	0.145033
13	N	-0.204888	0.501718
14	C	0.120853	0.114949
15	C	0.024664	-0.086256
16	C	-0.053722	-0.052878
17	C	0.071192	0.059460
18	N	-0.209848	-0.055204
19	C	-0.056665	-0.011673
20	H	0.111267	0.000525
21	C	0.110834	-0.146565
22	C	-0.040864	0.304300
23	H	0.137208	-0.013812
24	C	-0.038608	-0.155026
25	H	0.139341	0.006455
26	C	-0.029878	0.076285
27	H	0.139311	-0.003568
28	C	0.065980	0.305399
29	Cl	-0.137490	0.018221
30	O	-0.185000	-0.075826
31	C	0.265244	0.014065
32	O	-0.186572	-0.068595
33	C	-0.252719	-0.001658
34	H	0.121394	0.000471
35	H	0.117900	-0.000224
36	H	0.116784	-0.000504
37	Co	0.328242	1.143366
38	I	-0.061981	0.055591
39	I	-0.895525	0.004365

Sum of Mulliken charges = -0.00000 2.00000

Int6_T

Mulliken charges and spin densities:

		1	2
1	H	0.129449	0.002078
2	H	0.149211	-0.002677
3	C	-0.067256	0.004040

4	C	-0.000797	0.009720
5	C	-0.012344	-0.005930
6	C	-0.060038	0.003440
7	C	-0.058960	-0.006429
8	H	0.107572	-0.000160
9	H	0.115838	-0.000165
10	H	0.110352	0.000286
11	C	0.251315	-0.065790
12	O	-0.152996	0.122035
13	N	-0.204754	0.487337
14	C	0.113556	0.088757
15	C	0.019870	-0.071234
16	C	-0.061498	-0.048394
17	C	0.064657	0.056033
18	N	-0.202688	-0.048891
19	C	-0.055004	-0.007355
20	H	0.110448	0.000356
21	C	0.103699	-0.137742
22	C	-0.050673	0.252980
23	H	0.130204	-0.011461
24	C	-0.042565	-0.124754
25	H	0.133977	0.005250
26	C	-0.036907	0.066118
27	H	0.133511	-0.003075
28	C	0.057654	0.232793
29	Cl	-0.159184	0.011308
30	O	-0.180516	0.221578
31	C	0.255081	-0.011523
32	O	-0.185259	-0.094790
33	C	-0.250997	0.004472
34	H	0.113983	-0.000308
35	H	0.109540	-0.000911
36	H	0.109577	0.000684
37	Co	0.195675	1.045927
38	I	-0.116940	0.009578
39	I	-0.615793	0.016818

Sum of Mulliken charges = -0.00000 2.00000